B22

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
20 September 2001 (20.09.2001)

PCT

(10) International Publication Number
WO 01/68861 A2

(51) International Patent Classification[7]: C12N 15/13, C07K 16/00, C12N 15/86, 5/10, G01N 33/53, A61P 37/08, A61K 39/395, 31/00

(21) International Application Number: PCT/US01/08523

(22) International Filing Date: 15 March 2001 (15.03.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/189,403 15 March 2000 (15.03.2000) US
60/234,877 22 September 2000 (22.09.2000) US

(71) Applicant *(for all designated States except US)*: **NORTHWESTERN UNIVERSITY** [US/US]; 633 Clark Street, Evanston, IL 60201 (US).

(72) Inventors; and
(75) Inventors/Applicants *(for US only)*: **JARDETZKY, Theodore, S.** [US/US]; 7518 N. Eastlake Terrace, Chicago, IL 60626 (US). **WURZBURG, Beth, A.** [US/US]; 2544 Prairie Ave., No 33, Evanston, IL 60201 (US).

(74) Agents: **VERSER, Carol, Talkington** et al.; Heska Corporation, 1613 Prospect Parkway, Fort Collins, CO 80525 (US).

(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.

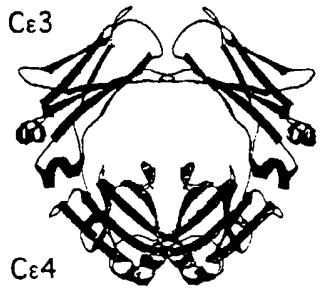
(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *without international search report and to be republished upon receipt of that report*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

WO 01/68861 A2

(54) Title: THREE-DIMENSIONAL MODEL OF A Fc REGION OF AN IgE ANTIBODY AND USES THEREOF



Closed
IgE-Fc

(57) Abstract: The present invention includes three-dimensional models of antibodies, such as Fc-Cε3/Cε4 regions of IgE antibodies, as well as methods to produce such models. The present invention also includes muteins having increased stabiltiy and/or antibody receptor binding activity, as well as methods to produce such muteins, preferably using information derived from three-dimensional models of the present invention. Also included are nucleic acid sequences encoding muteins of the present invention and use of those sequences to produce such muteins. Also included is the use of themodel to identify compounds that inhibit the binding of an antibody receptor protein to an antibody. The present invention also includes uses of such muteins and inhibitory compounds, for example, in methods to diagnose and protect animals from allergy and othter abnormal immune responses.

THREE-DIMENSIONAL MODEL OF A Fc REGION OF AN IgE ANTIBODY AND USES THEREOF

FIELD OF THE INVENTION

The present invention relates to a crystal and a three-dimensional (3-D) model of a constant region of an IgE antibody that includes the Cε3 and Cε4 domains (Fc-Cε3/Cε4, or Fc-Ce3/Ce4, region). The present invention also relates to the use of that model to produce muteins and inhibitors useful in the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

BACKGROUND OF THE INVENTION

Antibody Fc-receptors (FcRs) play an important role in the immune response by coupling the specificity of secreted antibodies to a variety of cells of the immune system. A number of cell types, including macrophages, mast cells, eosinophils, and basophils, express membrane-bound FcRs at their surfaces. The binding of antibodies to FcRs provides antigen-specificity to these cells, which upon activation release further cell-specific mediators of the immune response, such as interleukins, initiators of inflammation, leukotrienes, prostaglandins, histamines, or cytotoxic proteins. The adoptive specificity of the FcRs allows a combinatorial approach to pathogen elimination, by coupling the diversity of antibody antigen-recognition sites to the variety of cell-types expressing these receptors.

FcR-initiated mechanisms are important in normal immunity to infectious disease as well as in allergies, antibody-mediated tumor recognition, autoimmune diseases, and other diseases in which immune responses are abnormal (i.e., not regulated). Recent experiments with transgenic mice have demonstrated that the FcRs control key steps in the immune response, including antibody-directed cellular cytotoxicity and inflammatory cascades associated with the formation of immune complexes; see, for example, Ravetch et al., 1998, *Annu Rev Immunolo 16*, 421-432. Receptors that bind IgG (FcgRI, FcgRII, and FcgRIII, known collectively as FcgRs) mediate a variety of inflammatory reactions, regulate B-cell activation, and also trigger hypersensitivity reactions. The high affinity Fc epsilon receptor (also known as the IgE receptor or FceRI) is associated with the activation of mast cells and the triggering of

allergic reactions and anaphylactic shock. Knockout mice for the FceRI alpha chain (FcεRIα) are unable to mount IgE-mediated anaphylaxis (see for example, Dombrowicz et al., 1993, *Cell 75*, 969-976), although FcgRs are still able to activate mast cells (see, for example, Dombrowicz et al., 1997, *J. Clin. Invest. 99*, 915-925; Oettgen et al., 1994, *Nature 370*, 367-370). FceRI has also been shown to trigger anti-parasitic reactions from platelets and eosinophils as well as deliver antigen into the MHC class II presentation pathway for the activation of T cells; see, for example, Gounni et al., 1994, *Nature 367*, 183-186; Joseph et al., 1997, *Eur. J. Immunol. 27*, 2212-2218; Maurer et al., 1998, *J. Immunol. 161*, 2731-2739. The beta subunit of FceRI has been associated with asthma in genetic studies; see, for example, Hill et al., 1996, *Hum. Mol. Genet. 5*, 959-962; Hill et al., 1995, *Bmj 311*, 776-779; Kim et al., 1998, *Curr. Opin. Pulm. Med. 4*, 46-48; Mao et al., 1998, *Clin. Genet. 53*, 54-56; Shirakawa et al., 1994, *Nat. Genet. 7*, 125-129. A significant fraction of the population (~20%) may be affected by allergies, and this century has seen a substantial increase in asthma. Since IgE binding to FceRI is a requisite event in the reaction to different allergens, therapeutic strategies aimed at inhibiting FceRI could provide a useful treatment for these diseases. For example, monoclonal antibodies that target IgE and block receptor binding have shown therapeutic potential; see, for example, Heusser et al., 1997, *Curr. Opin. Immunol. 9*, 805-813.

FceRI is found as a tetrameric (abg_2) or trimeric (ag_2) membrane bound receptor on the surface of mast cells, basophils, eosinophils, langerhans cells and platelets. The alpha chain, also referred to as FcεRIα, of FceRI binds IgE molecules with high affinity (K_D of about 10^{-9} to 10^{-10} moles/liter (M)), and can be secreted as a 172-amino acid soluble, IgE-binding fragment by the introduction of a stop codon before the single C-terminal transmembrane anchor; see, for example, Blank et al.,1991, *E. J. Biol. Chem. 266*, 2639-2646, which describes the secretion of a soluble IgE-binding fragment of 172 amino acids. The extracellular domains of the human FcεRIα protein belong to the immunoglobulin (Ig) superfamily and contain seven N-linked glycosylation sites. Glycosylation of FcεRIα affects the secretion and stability of the receptor, but is not required for IgE-binding; see, for example, LaCroix et al., 1993, *Mol. Immunol. 30*,

321-330; Letourneur et al.,1995, *J. Biol. Chem. 270,* 8249-8256; Robertson, 1993, *J. Biol. Chem. 268*, 12736-12743; Scarselli et al., 1993, *FEBS Lett 329*, 223-226. The beta and gamma chains of FceRI are signal transduction modules.

Prior investigators have disclosed the nucleic acid sequence for human FcεRIα; see, for example, U.S. Patent No. 4,962,035, by Leder, issued October 9, 1990; U.S. Patent No. 5,639,660, by Kinet et al., issued June 17, 1997; Kochan et al., 1988, *Nucleic Acids Res. 16*, 3584; Shimizu et al., 1988, *Proc. Natl. Acad. Sci. USA 85*, 1907-1911; and Pang et al., 1993, *J. Immunol. 151*, 6166-6174. Nucleic acid sequences have also been reported for the human FceRI beta and gamma chains; see, respectively, Kuster et al., 1992, *J. Biol. Chem. 267*, 12782-12787; Kuster et al., 1990, *J. Biol. Chem. 265*, 6448-6452. Nucleic acid sequences have also been reported for nucleic acid molecules encoding canine FcεRIα, murine FcεRIα, rat FcεRIα, feline FcεRIα and equine FcεRIα proteins; see, respectively, GenBank™ accession number D16413; Swiss-Prot accession number P20489 (represents encoded protein sequence); GenBank accession number J03606; PCT Publication No. WO 98/27208, by Frank et al., published June 25, 1998, referred to herein as WO 98/27208; and PCT Publication No. WO 99/38974, by Weber et al., published August 5, 1999, referred to herein as WO 99/38974. In addition, methods to detect IgE antibodies using a FcεRIα protein have been reported in PCT Publication No. WO 98/23964, by Frank et al., published June 4, 1998, referred to herein as WO 98/23964; WO 98/27208, *ibid.*; PCT Publication No. WO 98/45707, by Frank et al., published October 15, 1998, referred to herein as WO 98/45707; and WO 99/38974, *ibid.*. WO 98/23964, WO 98/27208, WO 98/45707 and WO 99/38974 are each incorporated by reference herein in its entirety.

There have been several reports of the use of mutagenesis and swapping techniques to attempt to identify amino acids of either FcεRIα or IgE involved in the binding of (i.e., interaction between) those respective proteins, reports attempting to model FcεRIα proteins based on homology to other Ig-superfamily members, and reports that identify compounds that apparently inhibit such binding; see, for example, Cook et al., 1997, *Biochemistry 36*, 15579-15588; Hulett et al., 1994, *J. Biol. Chem. 269*, 15287-15293; Hulett et al., 1995, *J. Biol. Chem 270*, 21188-21194; Mallamaci et al.,

1993, *J. Biol. Chem. 268*, 22076-22083; Robertson, 1993, *ibid.*; Scarselli et al., 1993, *ibid.* McDonnell et al., 1997, *Biochem. Soc. Trans. 25*, 387-392; McDonnell et al., 1996, *Nat. Struc. Biol. 3*, 419-426; PCT Publication No. WO 97/40033, by Cheng et al., published October 30, 1997; U.S. Patent No. 5,180,805, by Gould et al, issued January 19, 1993; U.S. Patent No. 5,693,758, by Gould et al., issued December 2, 1997; PCT Publication No. WO 96/01643, by Gould et al., published January 25, 1996; PCT Publication No. WO 95/14779, by Gould et al., published June 1, 1995. None of these references, however, describe isolated crystals of FcεRIα proteins or 3-D models derived from crystals.

Despite what is known about FcRs and their interaction with antibodies, there remains a need for FcRs and antibodies with improved characteristics, such as enhanced affinity for their ligands, altered substrate specificity, increased stability, and increased solubility for use in diagnosis, treatment and prevention of allergy and other abnormal immune responses. Also needed for safe and efficacious compounds to prevent or treat allergy and to regulate other immune responses in an animal.

SUMMARY OF THE INVENTION

The present invention includes an isolated crystal of a constant region (Fc region) of an antibody, a three-dimensional (3-D) model of such a crystal and a modification of such a model. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as antibody muteins and other modified antibodies. Also included in the present invention are methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins. As such, the present invention includes antibodies with improved functions such as increased stability, increased affinity for an Ig binding domain of a FcR, altered substrate specificity, and increased solubility, including but not limited to reduced aggregation. Such proteins, also referred to as muteins, are useful to detect allergy and other immune response abnormalities as well as to protect an animal from such abnormalities. The present invention also provides safe and efficacious inhibitory compounds to protect (e.g., prevent, treat, reduce the consequences of) an animal from allergy and to regulate other immune responses in an animal.

The present invention includes a 3-D model of a human IgE Fc region comprising Cε3 and Cε4 domains, wherein the model substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3. The present invention also includes a 3-D model comprising a modification of a model substantially representing the atomic coordinates specified in Table 1, Table 2 or Table 3. Also included in the present invention are methods to produce such models.

The present invention also includes an isolated crystal of a human IgE Fc region comprising Cε3 and Cε4 domains.

The present invention includes a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein. The method includes the step of using a 3-D model of the present invention, and particularly one substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3. Also included in the present invention are inhibitory compounds identified using such a method. Also included are therapeutic compositions that include such inhibitory compounds and methods to use such therapeutic compositions to protect an animal from allergy or to regulate other immune responses (e.g., protect an animal from other abnormal immune responses).

The present invention also includes a mutein that binds to a Fc binding domain of a FcR. Such a mutein has an improved function compared to a protein that includes SEQ ID NO:2. Examples of such an improved function include increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, decreased aggregation, and increased solubility. Such a mutein is produced by a method that includes the following steps: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 2, or Table 3 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect an improved function of the protein; and (b) replacing the identified amino acid(s) to produce the mutein having such an improved function. The present invention also includes a mutein having an improved function compared to an unmodified IgE Fc region.

Also included are muteins that are chemically modified IgE Fc regions. Also included are nucleic acid molecules that encode muteins of the present invention, recombinant molecules and recombinant cells including such nucleic acid molecules and methods to produce such muteins. Also included are diagnostic reagents and diagnostic kits including such muteins, therapeutic compositions including such muteins, and methods to detect or protect an animal from allergy or other abnormal immune responses.

The present invention also includes a method to improve a function of a IgE Fc region which includes the steps of: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 2 or Table 3 to identify at least one amino acid of the protein which if replaced by a specified amino acid improves at least one of the functions of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having at least one of the improved functions.

BRIEF DESCRIPTION OF DRAWINGS

Fig. 1 shows a side-view comparison of the unbound IgE-Fc, receptor-bound IgE-Fc and IgG-Fc structures. The N-terminal domains are shown in blue. Fig. 1a shows the closed form of IgE-Fc Cε3-Cε4 domains. Fig. 1b shows the open form of IgE-Fc Cε3-Cε4 domains. Fig. 1c shows unbound IgG-Fc.

Fig.2 is a top-view comparison of the unbound IgE-Fc, receptor-bound IgE-Fc and IgG-Fc structures (N-terminal domains). β-strands are labeled (A-G) and a line is drawn between the first residue of the A strands for each Fc structure. In the closed IgE confirmation, this distance is 13 Å, in the open form it is 23 Å and in the IgG-Fc structure it is 22 Å. Fig. 2a shows the closed form of IgE-Fc Cε3-Cε4 domains. Fig. 2b shows the open form of IgE-Fc Cε3-Cε4 domains. Fig. 2c shows unbound IgG-Fc.

Fig. 3 shows a superposition of nine crystallographically independent IgG-Fc structures (grey/blue) with the open (dark blue) and closed (red) IgE-Fc structures. The IgG and IgE Fc structures were superimposed using Cα carbons from the C-terminal domain (Cγ2 or Cε3). IgG-Fc structures were used from the PDB files 1IGT, 1FC1, 1 FC2, 1FCC, 1IGY and 1ADQ. The 1MCO hinge-deleted antibody structure was not included in this analysis since it exhibits anomalous domain pairing throughout the protein structure. An asterisk is placed next to residue 366 in the BC loop of the IgE-Fc.

Fig. 4a shows a DynDom analysis of the domain motions characterizing the structural differences between bound and free IgE-Fc. One-half of an Fc (c3/c4 monomer) is shown in the closed conformation with the axis of the bend indicated by the dark red line. DynDom was used to determine the location of the axis and to calculate the change in the angle. Hinge residues (343-345, 351-352, and 435-436) are outlined in light purple. Residues that remain relatively fixed in both the open and closed forms of the Fc include the entire Cε4 domain, the interdomain linker, and the AB helix of Cε3. Residues in the Cε3 domain move as a semi-rigid domain. Fig. 4b shows a closeup of the residues at the Cε3/Cε4 and Cγ2/Cγ3 interfaces. IgG-Fc (red) (from pdb files 1IGT) and the closed IgE-Fc (blue) were superimposed using residues in the C-terminal domain (Cγ3 or Cε4). Note the displacement of the IgE-Fc helix (blue cylinder) away from the interdomain interface and the close approach of Cε3 residues to the IgG-Fc helix. The interactions of the AB helix with both domains may determine the full range of mobility of different antibody Fc domains. Fig.4c shows a graph of the residue displacements observed for both chains of the IgE-Fc in the free and receptor-bound crystal structures. One chain is shown with red circles, the other with blue diamonds. The Cα distances between amino acid residues in each structure was calculated after superposition of the two structures based on the alignment of the two Cε4 domains. Loops involved in binding receptor are indicated and highlighted in yellow and move by approximately 6-14 Å in the free form. "N" indicates Cε3 A strand residues, "C" is the carboxy terminus, "L" identifies the poorly ordered Cε4 AB loop, and "X" identifies a difference due to crystal contacts.

Fig. 5a shows a surface representation of the Cε3 and Cε4 domains (top-view) in the closed (left) and open (right) IgE-Fc structures. Receptor binding residues are shown in magenta and are from the Cε3 BC, DE and FG loops. Fig. 5b shows a side-view of the Cε3 and Cε4 domains described in Fig.5a.

Fig. 6 illustrates potential roles for IgE conformational changes in receptor-binding and structure-based inhibitor design. Open forms of the IgE molecule can interact with the high-affinity receptor (FcεRI), as shown by the crystal structure of the complex. IgE also binds to a low-affinity receptor, which is a trimer of C-type lectin domains (FceRII). FceRII could potentially interact with the closed form of the IgE

structure as shown in the upper left hand portion of the figure. The lectin domains are shown in blue while the IgE-Fc Cϵ3 domains are shown in yellow. Only two of the three lectin domains are thought to interact with the IgE. Three distinct classes of inhibitors of the IgE interaction are also shown on the left hand side of the figure. One class could bind to the open IgE and compete for FceRI-binding sites (competitive, lower left). Another class could bind to a region of IgE near the Ce3/Ce4 hinge and stabilize the closed form of IgE, thus inhibiting FceRI binding indirectly (allosteric inhibitor, center left). A third class of inhibitors could interact with FceRI-binding regions of the IgE, but stabilize a closed form of the IgE, acting as both a competitive and conformational inhibitor of FceRI binding (conformational inhibitor, center left).

Fig. 7a depicts the general structure of the IgG and IgE antibodies. Both antibodies contain two isotype-specific heavy chains and two light chains (H_2L_2). The Fab domains contain both heavy and light chain components while the Fc domains (shaded pink) are derived exclusively from the light chains. The IgE-Fc contains an extra domain pair (Cε2) compared to the IgG-Fc. The IgE Cε3-Cε4 domains are homologous to the IgG Cγ2-Cγ3 domains. Fig. 7b shows a structure-based sequence alignment of human IgE-Fc Cε3-Cε4 with the sequences of four IgG-Fc's for which crystal structure have been solved. IgE secondary structure is indicted using arrows for β-strands and ribbons for α-helices. Color bars indicate hinge residues (blue), FcεRi-binding loops (pink) and carbohydrate attachment sites (green dots). Within the sequence alignment, conserved residues are indicated with light-blue shading while structural differences (insertions, deletions, changes in secondary structure) between the IgG and IgE are highlighted in yellow. In addition, the completely conserved Cγ2 AB helix histidine residue (H310 in Igg1, H329 in IgG2a) and the corresponding residue in IgE, threonine 409, are indicated in yellow and pink respectively. The IgE numbering (above the sequence) is according to Dorrington and Bennich. The numbering of human IgG1 is given directly below the sequence. The PDB numbering of murine IG2a (1IGT), is shown in italics at the bottom (note that there are deletions in this numbering system).

Fig. 8a shows a side-view comparison of the unbound IgE-Fc, receptor-bound IgE-Fc and IgG-Fc structures. The N-terminal domains are shown in blue. Fig. 8b is a top-view comparison of the unbound IgE-Fc, receptor-bound IgE-Fc and IgG-Fc

structures (N-terminal domains). β-strands are labeled (A-G) and a line is drawn between the first residue of the A strands for each Fc structure. In the closed IgE confirmation, this distance is 13 Å, in the open form it is 23 Å and in the IgG-Fc structure it is 22 Å.

Fig. 9a shows a superposition of nine crystallographically independent IgG-Fc structures (grey/blue) with the open (dark blue) and closed (red) IgE-Fc structures. The IgG and IgE Fc structures were superimposed using Cα carbons from the C-terminal domain (Cγ2 or Cε3). IgG-Fc structures were used from the PDB files 1IGT, 1FC1, 1 FC2, 1FCC, 1IGY and 1ADQ. An asterisk is placed next to residue 366 in the BC loop of the IgE-Fc. Note the displacement of the IgE-Fc helix away from the interdomain interface, the movement of the IgE-Fc EF helix in the closed conformation, and the close approach of the IgG-Fc AB and EF helices at the site of the IgG residue insertion. Fig. 9b shows a DynDom analysis of the IgG-Fc. A stereo view of one chain of the Fc (closed conformation) is shown with the rotation axis indicated by an arrow. Hinge residues (343-345, 351-352, and 435-436) are outlined in cyan. Cε3 domain residues that move as a semi-rigid domain are shown in red. Residues that remain relatively fixed in both the open and closed forms of the Fc are shown in blue. Fig. 9c shows a DynDom analysis of three IgG-Fc structures. Shown is a stereo view with the rotation axes and hinge residues for murine IgG1 (1IGY) (cyan), murine IgG2a (1IGT) (purple) and human IgG1 (1FC1) (pink) on the Cα trace of the IgG2a structure. Fig. 9d shows the change in Cα coordinates between the closed and open conformations of the IgE-Fc. One chain is shown with red circles, the other with blue diamonds. Receptor binding loops are indicated and highlighted in pink; hinge residues are shown in cyan. "N" indicates Cε3 A strand residues, "C" is the carboxy terminus, "L" identifies the poorly ordered Cε4 AB loop, and "X" identifies a difference due to crystal contacts.

Fig. 10a diagrams the contacts made by the AB helix residues 9IgE Cε3 or IgG Cγ2). Residues of the AB and EF helices are shown on the grey helical wheels while the residues of the lower domain (Cε3 or Cε4) are shown below (blue lettering in blue ovals). Upper domain contacts (to Cε3 or Cγ2) involve residues in the EF helix and residues immediately adjacent to the AB helix. Lower domain contacts (to Cε4 or Cγ3) involve residues from the C, C', F and G β-sheet strands and the FG loop. Contacts

formed only in the open form of the IgE-Fc are indicated by dashed blue lines; the single contact formed only in the closed form is indicated by a red line. Contacts made by the conserved H329 in IgG are indicated by solid blue lines. The completely conserved EF helix H329 residue and the insertion residue I266 that forms a bulge just after the AB helix, are shown in yellow. Fig. 10b shows a surface representation of the interaction of EF helix residue T407 with the AB helix in the closed IgE-Fc while Fig. 10c shows this same interaction in the open IgE-Fc. Fig. 10d shows a surface representation of the packing interactions of the corresponding residue, the conserved h329, in IgG-Fc, with the bulge a the C-terminus of the Cγ2 AB helix.

Fig. 11a shows a molecular surface representation of the Cϵ3 and Cϵ4 domains (side-view) in the closed (left) and open (right) IgE-Fc structures. Receptor binding residues are shown in magenta and are from the Cϵ3 BC, DE and FG loops. Fig. 11b shows a top-view of the Cϵ3 and Cϵ4 domains described in Fig.11a.

Fig. 12 shows possible roles for IgE flexibility in Fc receptor binding and structure-based inhibitor design. The Cε3 domains are colored to correspond to the different conformational states, open (pink) and closed (yellow); the Cε4 domains are shown in grey. Open forms of the IgE molecule can bind to the high affinity receptor, FcεRI. The low affinity receptor, FcεRII, is a trimeric C-type lectin that binds to an unidentified conformation of the IgE-Fc (green). Three potential classes of inhibitors of the IgE:FcεRI interactions are shown: binding site competitive inhibitor, binding sire conformational inhibitor, and allosteric conformational inhibitor.

Fig. 13 illustrates a potential drug binding site near the IgE-Fc hinge. A hypothetical drug (green) is shown inside the hinge cavity. Residues surrounding the cavity include R342, P343, S344, P3435, L348, W410, I411, K435, T436, R440,P471, E472, D473, E529.

DETAILED DESCRIPTION OF THE INVENTION

The present invention includes isolated crystals of Fc regions of antibodies, 3-D models of such crystals and modifications of such models. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as muteins and other modified antibodies. Also included in the present invention are

methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins.

The present invention includes an isolated crystal of a Fc region comprising the Cε3 and Cε4 domains of an IgE antibody (Fc-Cε3/Cε4), a 3-D model of such a crystal and a modification of such a model. As used herein, the term "a" entity or "an" entity refers to one or more of that entity; for example, a crystal or a model refers to one or more crystals or models, respectively. As such, the terms "a" (or "an"), "one or more" and "at least one" can be used interchangeably herein. It is also to be noted that the terms "comprising", "including", and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures, or combinations, of two or more of the compounds.

As used herein, an extracellular domain of a FcεRIα protein is the portion of the FceRI alpha chain that is exposed to the environment outside the cell and that binds to the Fc domain of an IgE antibody. Such an extracellular domain can be (a) a complete extracellular domain which is a domain that extends from the first amino acid of a mature FceRI alpha chain through the last amino acid prior to the start of the transmembrane region or a domain that is functionally equivalent, in that such a domain includes a D1 and D2 domain, displays a similar affinity for the IgE antibody to which such an FcεRIα protein naturally binds, and produces crystals having sufficient quality to enable structure determination, or (b) a fragment of any of the extracellular domains of (a), wherein the fragment retains its ability to bind to the Fc domain of an antibody. As used herein, the terms binding to an antibody and binding to the Fc domain (i.e., constant region) of an antibody can be used interchangeably since it is recognized that a FcR binds to the Fc domain of an antibody. A FcR (i.e., a protein that can bind to an antibody), such as a FcεRIα protein, can be a full-length FcR (e.g., a full-length FceRI alpha chain), or any fragment thereof, wherein the fragment binds to an antibody. Similarly an antibody, or an Fc region thereof, can be a full-length antibody, or full-length Fc region thereof, or any fragment thereof that binds to a FcR. In one embodiment an Fc region comprises Cε3 and Cε4 domains. Preferably a FcR binds to

an antibody with an affinity (K_A) of at least about 10^8 liters/mole (M^{-1}), more preferably of at least about $10^9 M^{-1}$, and even more preferably of at least about $10^{10} M^{-1}$.

The present invention is surprising in several aspects. For example, this is the first report of an isolated crystal of a Fc-Cε3/Cε4 region of an IgE antibody, and in particular of an isolated crystal of sufficient quality that a crystal structure, i.e., a 3-D model, could be derived therefrom. Generation of such a crystal was very difficult and non-obvious and has been attempted by others without success. The inventors tried many approaches before discovering a preferred Fc-Cε3/Cε4 region from which to make a useful crystal. The first such region to be used successfully is referred to herein as PhFc-Cε3/Cε4_{1-222} which is composed of the four amino acids alanine, aspartic acid, proline and cysteine at the amino terminus followed by amino acids 330 through 547 of the human IgE Fc constant region, using the numbering system of Dorrington et al, 1978, *Immunol Rev 41*, 3-25. PhFc-Cε3/Cε4_{1-222} is represented herein by SEQ ID NO:2. An example of a nucleic acid molecule encoding PhFc-Cε3/Cε4_{1-222} is referred to herein as nhFc-Cε3/Cε4_{1-666}, the nucleic acid sequence of which is referred to herein as SEQ ID NO:1. It was also discovered that better crystals are generated when PhFc-Cε3/Cε4_{1-222} is produced in insect cells, using a method such as that described in the Examples. Solution of the crystal structure was also very difficult, as described in more detail in the Examples. For example, as part of the effort, approximately 12,000 models were generated and used in complete Molecular Replacement searches with the program Amore, taking about 10 days on 5 Silicon Graphics computers.

Determination of the crystal structure of PhFc-Cε3/Cε4_{1-222} produced in *Trichoplusia ni* (Hi-5) cells resulted in a 3-D model that substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3. Amino acids are represented herein by their standard three or one letter codes; see, for example, Sambrook et al., *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Labs Press, 1989, which is incorporated herein by reference in its entirety.

The 3-D model of PhFc-Cε3/Cε4_{1-222} is also very surprising in view of what is known about the crystal structure of the Fc region of IgG. The Fc region of IgE exists in a novel conformation that is more compact than that of IgG. The Cε3 domains are also

much closer to each other in IgE compared to IgG (about 13 angstroms compared to about 22 angstroms), leading to the descriptor of "closed conformation" for the IgE Fc structure. This closed conformation is also surprising in view of the crystal structures of FcεRIα alone, which is disclosed in U.S. Patent Application Serial No. 09/434,193, filed November 4, 1999, by Jardetzky et al., and in PCT Publication No. WO 00/26246, published May 11, 2000, by Jardetzky et al., and of the complex between FcεRIα and Fc-Cε3/Cε4 alone, which is disclosed in U.S. Patent Application Serial No. 60/189,853. US 09/434,193, *ibid.*, WO 00/26246, *ibid.* and 60/189,853, *ibid.*, are incorporated by reference herein in their entireties. The structure of Fc-Cε3/Cε4 in the complex is an open conformation, also referred to as a receptor-bound conformation. The distance between the two Cε3 domains in the receptor-bound conformation is about 23 angstroms. Comparison of these structural similarities and differences are described in greater detail in the Examples and in 60/189,853, *ibid.* Analysis of the model which substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3 indicates the necessity of such a model for proper interpretation and refinement of mutagenesis studies that have been reported. Such a model permits differentiation between amino acids directly or indirectly influencing binding of FcεRIα to IgE and demonstrates where amino acids and amino acid segments identified in mutagenesis studies are positioned on the protein. By using a model of the present invention one can identify the interactions of FcεRIα and IgE, thereby identifying amino acids to target for mutein production or regions to target for the development of compounds to inhibit binding of IgE to its receptor. Such a model also leads to the ability to design inhibitory compounds that stabilize the closed conformation of IgE, thereby reducing its ability to bind to a FcR. Such a model can be used alone or in conjunction with a model of FcεRIα alone (US 09/434,193, *ibid.* and WO 00/26246, *ibid.*) or of the complex between FcεRIα and Fc-Cε3/Cε4 alone (60/189,853, *ibid.*).

One embodiment of the present invention is an isolated crystal of a Fc-Cε3/Cε4 region of an IgE antibody. As used herein, an isolated crystal is a crystal of a protein that has been produced in a laboratory; that is, an isolated crystal is produced by an individual and is not an object found *in situ* in nature. It is appreciated by those skilled

in the art that there are a variety of techniques to produce crystals including, but not limited to, vapor diffusion using a hanging or sitting drop methodology, vapor diffusion under oil, and batch methods; see, for example, Ducruix et al., eds., 1991, *Crystallization of nucleic acids and proteins; A practical approach*, Oxford University Press, and Wyckoff et al., eds., 1985, *Methods in Enzymology 11*, 49-185; each reference is incorporated by reference herein in its entirety. It is also to be appreciated that crystallization conditions can be adjusted depending on a protein's inherent characteristics as well as on a protein's concentration in a solution and that a variety of precipitants can be added to a protein solution in order to effect crystallization; such precipitants are known to those skilled in the art. In a preferred embodiment, a crystal of a Fc-Cε3/Cε4 region is produced in a solution by adding a precipitant such as polyethylene glycol (PEG) or PEG monomethylether. It is also to be noted that a Fc-Cε3/CCε4 region used to produce a crystal can be produced by a variety of methods, including purification of a native protein, chemical synthesis of a protein, or recombinant production of a protein. Although a number of cell types can be used to recombinantly produce such a protein, insect cells, such as, but not limited to *Trichoplusia ni* and *Spodoptera frugiperda*, are preferred, with *Trichoplusia ni* cells being more preferred. Additional methods to produce proteins are disclosed below.

Isolated crystals of the present invention can include heavy atom derivatives, such as, but not limited to, gold, platinum, mercury, selenium, copper, and lead. Such heavy atoms can be introduced randomly or introduced in a manner based on knowledge of 3-D models of the present invention. Additional crystals of the present invention are not derivatized. In one embodiment, an isolated crystal of the present invention is a co-crystal of a FcεRIα protein bound to a Fc domain of an IgE antibody in the presence of a compound that inhibits the binding of a FcεRIα protein to a Fc domain of an IgE antibody. Additional crystals of the present invention include crystals produced from proteins that are muteins of the present invention or other proteins that are represented by a 3-D model of the present invention.

An isolated crystal of the present invention can be the crystal of any suitable Fc region that binds to FcεRIα, such as a Fc comprising Cε3 domains or a Fc comprising

Cε3 and Cε4 domains. Suitable Fc-Cε3/Cε4 regions include mammalian Fc-Cε3/Cε4 regions, with human, canine, feline, equine, rat and murine Fc-Cε3/Cε4 regions being preferred, and human Fc-Cε3/Cε4 regions being even more preferred. A preferred crystal of the present invention diffracts X-rays to a resolution of about 4.5 angstroms or higher (i.e., lower number meaning higher resolution), with resolutions of about 4.0 angstroms or higher, about 3.5 angstroms or higher, about 3.25 angstroms or higher, about 3 angstroms or higher, about 2.5 angstroms or higher, about 2.3 angstroms or higher, about 2 angstroms or higher, about 1.5 angstroms or higher, and about 1 angstrom or higher being increasingly more preferred. It is appreciated, however, that additional crystals of lower resolutions can have utility in discerning overall topology of the structures, e.g., location of a binding site or where a molecule binds to a receptor or to an antibody. A particularly preferred isolated crystal of the present invention has amino acid sequence SEQ ID NO:2, or a sequence essentially equivalent that represents another mammalian Fc-Cε3/Cε4 region. Preferred are crystals that belong to spacegroup $P42_12$. Particularly preferred crystals include a crystal belonging to spacegroup $P42_12$ that has cell dimensions of 105.6 angstroms x 105.6 angstroms x 47.1 angstroms, alpha=beta=gamma=90 degrees and that contains one Cε3/Cε4 chain per asymmetric unit of the crystal. Such a preferred crystal preferably diffracts X-rays to a resolution of about 2.3 angstroms.

The present invention includes a 3-D model of a Fc-Cε3/Cε4 region that substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3. The present invention also includes 3-D models that comprise modifications of the model substantially represented by the atomic coordinates specified in Table 1, Table 2 or Table 3. Each such modification represents an antibody Fc region that binds to a Fc receptor protein. A 3-D model of a Fc-Cε3/Cε4 region is a representation, or image, that predicts the actual structure of the corresponding region. As such, a 3-D model is a tool that can be used to probe the relationship between the region's structure and function at the atomic level and to design muteins (i.e., genetically and/or chemically altered antibodies) having an improved function, such as, but not limited to: increased (i.e., enhanced) stability; increased FcR binding activity, for example, by, increasing the

affinity for an FcR by, for example, increasing the association rate and/or decreasing the dissociation rate between a FcR and an antibody or by altering substrate specificity (e.g., enhancing the ability of an Fc region of a certain species and class to bind to an antibody binding site from another species and/or another antibody class); and/or increased solubility (e.g., reduced aggregation). It is well known to those skilled in the art, however, that a 3-D model of a protein derived by analysis of protein crystals is not identical to the inherent structure of the protein. See, for example, Branden et al., *Introduction to Protein Structure*, Garland Publishing Inc., New York and London, 1991, especially on page 277, which states "not surprisingly the model never corresponds precisely to the actual crystal." Furthermore, the model can be subjected to further refinements to more closely correspond to the actual structure of a Fc region of an antibody. Such a refined model, which is an example of a modification of the present invention, is a better predictor of the actual structure and mechanism of action of the protein that the model represents. A refinement of a 3-D model of the present invention refers to an improved model of a Fc-Cε3/Cε4 region that can be obtained in a variety of ways known to those skilled in the art. Refinements can include models determined to more preferred degrees of resolution, preferably to about 4.5 angstroms, more preferably to about 4 angstroms, more preferably to about 3.5 angstroms, more preferably to about 3.25 angstroms, more preferably to about 3 angstroms, more preferably to about 2.5 angstroms, more preferably to about 2.3 angstroms, more preferably to about 2 angstroms, more preferably to about 1.5 angstroms, and even more preferably to about 1 angstrom. Preferred refinements are obtained using the 3-D model as a basis for such improvements.

One embodiment of the present invention is a 3-D model of a Fc-Cε3/Cε4 region that substantially represents the atomic coordinates specified (i.e., listed) in Table 1.

Table 1. Atomic coordinates of 7_more_dimer.pdb

ATOM #	ATOM TYPE	RES	CHN	#	X	Y	Z	OCC	b
1	CB	VAL	A	336	46.217	60.546	16.604	1.00	63.58
2	CG1	VAL	A	336	45.590	59.856	15.405	1.00	64.76
3	CG2	VAL	A	336	47.677	60.888	16.335	1.00	68.51
4	C	VAL	A	336	44.045	61.436	17.434	1.00	61.62
5	O	VAL	A	336	43.880	60.399	18.074	1.00	64.02
6	N	VAL	A	336	46.161	62.624	17.972	1.00	59.58
7	CA	VAL	A	336	45.438	61.827	16.943	1.00	61.95
8	N	SER	A	337	43.046	62.262	17.137	1.00	59.54
9	CA	SER	A	337	41.679	61.982	17.564	1.00	57.94
10	CB	SER	A	337	41.204	63.069	18.525	1.00	56.70
11	OG	SER	A	337	41.581	64.347	18.053	1.00	65.28
12	C	SER	A	337	40.697	61.833	16.400	1.00	56.67
13	O	SER	A	337	40.987	62.234	15.268	1.00	56.61
14	N	ALA	A	338	39.539	61.245	16.687	1.00	52.92
15	CA	ALA	A	338	38.521	61.011	15.671	1.00	51.01
16	CB	ALA	A	338	38.576	59.562	15.216	1.00	50.96
17	C	ALA	A	338	37.120	61.348	16.166	1.00	50.95
18	O	ALA	A	338	36.816	61.204	17.352	1.00	53.16
19	N	TYR	A	339	36.272	61.805	15.250	1.00	47.68
20	CA	TYR	A	339	34.903	62.169	15.592	1.00	48.08
21	CB	TYR	A	339	34.810	63.675	15.897	1.00	50.34
22	CG	TYR	A	339	35.892	64.218	16.817	1.00	58.74
23	CD1	TYR	A	339	37.196	64.421	16.355	1.00	60.22
24	CE1	TYR	A	339	38.199	64.895	17.205	1.00	64.78
25	CD2	TYR	A	339	35.616	64.506	18.153	1.00	60.49
26	CE2	TYR	A	339	36.608	64.980	19.012	1.00	63.00
27	CZ	TYR	A	339	37.900	65.172	18.533	1.00	67.92
28	OH	TYR	A	339	38.891	65.626	19.382	1.00	68.47
29	C	TYR	A	339	33.954	61.815	14.437	1.00	45.49
30	O	TYR	A	339	34.262	62.044	13.267	1.00	43.52
31	N	LEU	A	340	32.808	61.238	14.775	1.00	44.01
32	CA	LEU	A	340	31.816	60.872	13.776	1.00	42.54
33	CB	LEU	A	340	31.550	59.363	13.816	1.00	39.07
34	CG	LEU	A	340	30.652	58.750	12.730	1.00	39.58
35	CD1	LEU	A	340	31.198	59.074	11.349	1.00	28.76
36	CD2	LEU	A	340	30.571	57.236	12.923	1.00	35.57
37	C	LEU	A	340	30.557	61.645	14.134	1.00	42.53
38	O	LEU	A	340	30.138	61.638	15.286	1.00	43.25
39	N	SER	A	341	29.957	62.324	13.160	1.00	42.42
40	CA	SER	A	341	28.752	63.103	13.425	1.00	40.32
41	CB	SER	A	341	28.997	64.586	13.105	1.00	41.30
42	OG	SER	A	341	29.416	64.758	11.764	1.00	45.86
43	C	SER	A	341	27.563	62.606	12.634	1.00	38.67
44	O	SER	A	341	27.707	62.048	11.559	1.00	42.94
45	N	ARG	A	342	26.378	62.823	13.177	1.00	37.60
46	CA	ARG	A	342	25.155	62.414	12.520	1.00	35.91
47	CB	ARG	A	342	24.026	62.359	13.552	1.00	36.67
48	CG	ARG	A	342	24.254	61.315	14.646	1.00	39.89
49	CD	ARG	A	342	23.141	61.322	15.679	1.00	42.31
50	NE	ARG	A	342	23.185	62.534	16.490	1.00	45.87
51	CZ	ARG	A	342	24.005	62.730	17.520	1.00	52.30
52	NH1	ARG	A	342	24.861	61.790	17.895	1.00	56.74
53	NH2	ARG	A	342	23.981	63.885	18.168	1.00	58.22
54	C	ARG	A	342	24.832	63.409	11.398	1.00	34.19
55	O	ARG	A	342	25.476	64.450	11.278	1.00	34.44
56	N	PRO	A	343	23.837	63.101	10.555	1.00	31.22
57	CD	PRO	A	343	23.028	61.871	10.494	1.00	34.08

	58	CA	PRO	A	343	23.486	64.024	9.466	1.00	33.86
	59	CB	PRO	A	343	22.437	63.244	8.663	1.00	32.10
	60	CG	PRO	A	343	22.698	61.789	9.022	1.00	37.07
	61	C	PRO	A	343	22.897	65.323	10.015	1.00	32.54
	62	O	PRO	A	343	22.270	65.319	11.072	1.00	35.02
	63	N	SER	A	344	23.090	66.432	9.311	1.00	33.04
	64	CA	SER	A	344	22.515	67.687	9.778	1.00	34.74
	65	CB	SER	A	344	23.172	68.897	9.095	1.00	35.18
	66	OG	SER	A	344	22.663	69.093	7.792	1.00	35.70
	67	C	SER	A	344	21.038	67.628	9.415	1.00	35.17
	68	O	SER	A	344	20.669	67.132	8.349	1.00	32.53
	69	N	PRO	A	345	20.162	68.094	10.313	1.00	35.98
	70	CD	PRO	A	345	20.377	68.420	11.736	1.00	36.93
	71	CA	PRO	A	345	18.731	68.056	9.995	1.00	34.79
	72	CB	PRO	A	345	18.097	68.730	11.212	1.00	30.45
	73	CG	PRO	A	345	18.988	68.221	12.331	1.00	30.91
	74	C	PRO	A	345	18.385	68.739	8.667	1.00	34.13
	75	O	PRO	A	345	17.471	68.317	7.963	1.00	34.14
	76	N	PHE	A	346	19.124	69.783	8.309	1.00	31.57
	77	CA	PHE	A	346	18.848	70.466	7.059	1.00	33.19
	78	CB	PHE	A	346	19.711	71.724	6.935	1.00	37.49
	79	CG	PHE	A	346	19.616	72.394	5.595	1.00	38.65
	80	CD1	PHE	A	346	18.432	72.979	5.178	1.00	42.62
	81	CD2	PHE	A	346	20.719	72.441	4.747	1.00	43.21
	82	CE1	PHE	A	346	18.344	73.608	3.933	1.00	41.72
	83	CE2	PHE	A	346	20.643	73.069	3.496	1.00	49.00
	84	CZ	PHE	A	346	19.452	73.654	3.091	1.00	42.82
	85	C	PHE	A	346	19.099	69.530	5.867	1.00	33.37
	86	O	PHE	A	346	18.284	69.457	4.948	1.00	33.52
	87	N	ASP	A	347	20.216	68.810	5.884	1.00	32.94
	88	CA	ASP	A	347	20.533	67.891	4.792	1.00	33.61
	89	CB	ASP	A	347	21.962	67.358	4.927	1.00	29.68
	90	CG	ASP	A	347	23.011	68.378	4.541	1.00	35.85
	91	OD1	ASP	A	347	24.214	68.084	4.718	1.00	42.71
	92	OD2	ASP	A	347	22.646	69.472	4.056	1.00	50.58
	93	C	ASP	A	347	19.564	66.718	4.762	1.00	33.62
	94	O	ASP	A	347	19.201	66.219	3.699	1.00	30.10
	95	N	LEU	A	348	19.137	66.288	5.940	1.00	34.23
	96	CA	LEU	A	348	18.226	65.163	6.054	1.00	38.75
	97	CB	LEU	A	348	18.260	64.636	7.496	1.00	38.06
	98	CG	LEU	A	348	17.363	63.435	7.811	1.00	43.84
	99	CD1	LEU	A	348	17.739	62.243	6.910	1.00	39.77
	100	CD2	LEU	A	348	17.510	63.064	9.291	1.00	43.35
	101	C	LEU	A	348	16.763	65.439	5.645	1.00	39.57
	102	O	LEU	A	348	16.146	64.621	4.959	1.00	38.51
	103	N	PHE	A	349	16.214	66.583	6.057	1.00	40.41
	104	CA	PHE	A	349	14.809	66.901	5.762	1.00	42.87
	105	CB	PHE	A	349	14.111	67.364	7.040	1.00	39.59
	106	CG	PHE	A	349	14.208	66.383	8.163	1.00	37.95
	107	CD1	PHE	A	349	15.004	66.649	9.268	1.00	36.40
	108	CD2	PHE	A	349	13.517	65.181	8.105	1.00	40.49
	109	CE1	PHE	A	349	15.116	65.726	10.305	1.00	39.63
	110	CE2	PHE	A	349	13.619	64.247	9.135	1.00	38.12
	111	CZ	PHE	A	349	14.418	64.520	10.237	1.00	41.86
	112	C	PHE	A	349	14.472	67.896	4.654	1.00	44.67
	113	O	PHE	A	349	13.433	67.773	4.001	1.00	47.25
	114	N	ILE	A	350	15.314	68.895	4.450	1.00	46.06
	115	CA	ILE	A	350	15.027	69.871	3.417	1.00	50.35
	116	CB	ILE	A	350	15.548	71.270	3.813	1.00	50.30
	117	CG2	ILE	A	350	14.997	72.316	2.864	1.00	51.91
	118	CG1	ILE	A	350	15.146	71.593	5.261	1.00	51.78
	119	CD1	ILE	A	350	13.685	71.366	5.580	1.00	45.73

	120	C	ILE	A	350	15.694	69.421	2.127	1.00	51.95
	121	O	ILE	A	350	15.028	69.146	1.130	1.00	52.71
	122	N	ARG	A	351	17.016	69.319	2.173	1.00	53.39
	123	CA	ARG	A	351	17.813	68.909	1.031	1.00	54.67
	124	CB	ARG	A	351	19.290	69.059	1.393	1.00	59.14
	125	CG	ARG	A	351	20.186	69.537	0.267	1.00	64.87
	126	CD	ARG	A	351	21.254	70.473	0.808	1.00	66.51
	127	NE	ARG	A	351	22.405	70.566	-0.080	1.00	73.42
	128	CZ	ARG	A	351	23.263	69.573	-0.283	1.00	78.26
	129	NH1	ARG	A	351	23.094	68.417	0.344	1.00	81.30
	130	NH2	ARG	A	351	24.288	69.733	-1.111	1.00	79.63
	131	C	ARG	A	351	17.508	67.468	0.616	1.00	53.92
	132	O	ARG	A	351	17.510	67.144	-0.567	1.00	53.66
	133	N	LYS	A	352	17.248	66.612	1.598	1.00	53.41
	134	CA	LYS	A	352	16.942	65.200	1.360	1.00	53.02
	135	CB	LYS	A	352	15.779	65.053	0.375	1.00	54.25
	136	CG	LYS	A	352	14.506	65.752	0.814	1.00	64.61
	137	CD	LYS	A	352	13.366	65.442	-0.146	1.00	71.92
	138	CE	LYS	A	352	12.202	66.410	0.014	1.00	76.75
	139	NZ	LYS	A	352	12.573	67.793	-0.405	1.00	82.42
	140	C	LYS	A	352	18.130	64.383	0.847	1.00	51.14
	141	O	LYS	A	352	17.945	63.417	0.109	1.00	51.55
	142	N	SER	A	353	19.341	64.772	1.237	1.00	47.69
	143	CA	SER	A	353	20.552	64.067	0.832	1.00	45.50
	144	CB	SER	A	353	21.154	64.718	-0.418	1.00	50.28
	145	OG	SER	A	353	21.538	66.058	-0.171	1.00	63.45
	146	C	SER	A	353	21.528	64.135	2.006	1.00	40.39
	147	O	SER	A	353	22.498	64.890	1.995	1.00	40.20
	148	N	PRO	A	354	21.268	63.329	3.045	1.00	36.74
	149	CD	PRO	A	354	20.188	62.338	3.039	1.00	36.52
	150	CA	PRO	A	354	22.043	63.224	4.283	1.00	34.20
	151	CB	PRO	A	354	21.182	62.317	5.163	1.00	31.70
	152	CG	PRO	A	354	19.870	62.260	4.472	1.00	40.26
	153	C	PRO	A	354	23.433	62.636	4.121	1.00	32.13
	154	O	PRO	A	354	23.655	61.771	3.283	1.00	28.54
	155	N	THR	A	355	24.359	63.111	4.942	1.00	30.96
	156	CA	THR	A	355	25.718	62.601	4.936	1.00	31.86
	157	CB	THR	A	355	26.692	63.501	4.121	1.00	32.67
	158	OG1	THR	A	355	26.806	64.777	4.752	1.00	34.86
	159	CG2	THR	A	355	26.194	63.706	2.699	1.00	34.90
	160	C	THR	A	355	26.221	62.548	6.374	1.00	33.38
	161	O	THR	A	355	25.703	63.239	7.260	1.00	32.61
	162	N	ILE	A	356	27.197	61.691	6.618	1.00	32.83
	163	CA	ILE	A	356	27.793	61.641	7.935	1.00	33.21
	164	CB	ILE	A	356	27.538	60.303	8.666	1.00	34.88
	165	CG2	ILE	A	356	26.038	60.142	8.910	1.00	34.84
	166	CG1	ILE	A	356	28.098	59.135	7.860	1.00	37.26
	167	CD1	ILE	A	356	27.809	57.757	8.489	1.00	38.06
	168	C	ILE	A	356	29.265	61.855	7.639	1.00	32.48
	169	O	ILE	A	356	29.739	61.563	6.536	1.00	30.30
	170	N	THR	A	357	29.991	62.364	8.622	1.00	33.59
	171	CA	THR	A	357	31.389	62.671	8.406	1.00	32.83
	172	CB	THR	A	357	31.575	64.216	8.243	1.00	37.46
	173	OG1	THR	A	357	30.985	64.645	7.009	1.00	35.11
	174	CG2	THR	A	357	33.047	64.599	8.258	1.00	40.13
	175	C	THR	A	357	32.274	62.180	9.530	1.00	34.22
	176	O	THR	A	357	31.991	62.378	10.716	1.00	33.99
	177	N	CYS	A	358	33.369	61.555	9.134	1.00	34.04
	178	CA	CYS	A	358	34.344	61.037	10.068	1.00	36.90
	179	C	CYS	A	358	35.496	62.027	9.999	1.00	36.26
	180	O	CYS	A	358	36.103	62.188	8.944	1.00	35.68
	181	CB	CYS	A	358	34.809	59.670	9.593	1.00	39.83

	182	SG	CYS	A	358	35.781	58.719	10.798	1.00	52.73
	183	N	LEU	A	359	35.780	62.692	11.112	1.00	38.57
	184	CA	LEU	A	359	36.849	63.679	11.178	1.00	42.35
	185	CB	LEU	A	359	36.327	64.985	11.796	1.00	42.11
	186	CG	LEU	A	359	37.373	66.028	12.219	1.00	48.42
	187	CD1	LEU	A	359	38.221	66.454	11.027	1.00	49.46
	188	CD2	LEU	A	359	36.666	67.230	12.831	1.00	48.09
	189	C	LEU	A	359	38.011	63.163	12.005	1.00	45.39
	190	O	LEU	A	359	37.834	62.806	13.165	1.00	48.73
	191	N	VAL	A	360	39.195	63.121	11.407	1.00	47.72
	192	CA	VAL	A	360	40.395	62.669	12.104	1.00	51.87
	193	CB	VAL	A	360	41.086	61.525	11.335	1.00	52.99
	194	CG1	VAL	A	360	42.365	61.110	12.049	1.00	51.29
	195	CG2	VAL	A	360	40.144	60.348	11.210	1.00	52.42
	196	C	VAL	A	360	41.379	63.833	12.226	1.00	55.21
	197	O	VAL	A	360	41.634	64.537	11.247	1.00	56.01
	198	N	VAL	A	361	41.920	64.042	13.423	1.00	57.47
	199	CA	VAL	A	361	42.882	65.121	13.652	1.00	61.75
	200	CB	VAL	A	361	42.352	66.153	14.675	1.00	58.91
	201	CG1	VAL	A	361	43.389	67.232	14.913	1.00	56.98
	202	CG2	VAL	A	361	41.070	66.774	14.166	1.00	54.49
	203	C	VAL	A	361	44.197	64.555	14.177	1.00	66.78
	204	O	VAL	A	361	44.208	63.764	15.119	1.00	67.30
	205	N	ASP	A	362	45.301	64.959	13.556	1.00	72.35
	206	CA	ASP	A	362	46.631	64.500	13.955	1.00	79.16
	207	CB	ASP	A	362	47.334	63.825	12.769	1.00	83.66
	208	CG	ASP	A	362	48.603	63.089	13.176	1.00	87.40
	209	OD1	ASP	A	362	49.071	63.283	14.320	1.00	91.40
	210	OD2	ASP	A	362	49.138	62.318	12.348	1.00	87.33
	211	C	ASP	A	362	47.444	65.704	14.424	1.00	82.84
	212	O	ASP	A	362	47.937	66.487	13.607	1.00	84.14
	213	N	ALA	A	363	47.578	65.849	15.740	1.00	85.70
	214	CA	ALA	A	363	48.319	66.964	16.325	1.00	89.05
	215	CB	ALA	A	363	48.446	66.770	17.830	1.00	90.18
	216	C	ALA	A	363	49.701	67.142	15.699	1.00	91.80
	217	O	ALA	A	363	50.243	68.246	15.691	1.00	92.23
	218	N	ALA	A	364	50.263	66.056	15.174	1.00	94.23
	219	CA	ALA	A	364	51.578	66.085	14.536	1.00	97.42
	220	CB	ALA	A	364	52.668	66.159	15.594	1.00	96.05
	221	C	ALA	A	364	51.755	64.828	13.687	1.00	100.00
	222	O	ALA	A	364	51.767	63.715	14.213	1.00	101.29
	223	N	PRO	A	365	51.885	64.988	12.359	1.00	101.76
	224	CD	PRO	A	365	51.407	66.158	11.597	1.00	101.62
	225	CA	PRO	A	365	52.053	63.836	11.468	1.00	103.14
	226	CB	PRO	A	365	51.022	64.114	10.394	1.00	103.27
	227	CG	PRO	A	365	51.228	65.594	10.183	1.00	103.12
	228	C	PRO	A	365	53.456	63.681	10.872	1.00	104.03
	229	O	PRO	A	365	54.419	63.372	11.579	1.00	104.47
	230	N	ALA	A	366	53.536	63.884	9.557	1.00	104.37
	231	CA	ALA	A	366	54.776	63.793	8.793	1.00	104.87
	232	CB	ALA	A	366	55.839	64.705	9.413	1.00	105.36
	233	C	ALA	A	366	55.319	62.370	8.665	1.00	104.90
	234	O	ALA	A	366	56.461	62.108	9.045	1.00	105.14
	235	N	LYS	A	367	54.514	61.452	8.129	1.00	104.05
	236	CA	LYS	A	367	54.982	60.077	7.972	1.00	103.07
	237	CB	LYS	A	367	55.483	59.539	9.315	1.00	103.33
	238	CG	LYS	A	367	54.411	59.406	10.383	1.00	102.12
	239	CD	LYS	A	367	54.951	58.638	11.572	1.00	103.99
	240	CE	LYS	A	367	53.876	58.371	12.604	1.00	103.83
	241	NZ	LYS	A	367	54.417	57.544	13.714	1.00	105.88
	242	C	LYS	A	367	54.024	59.046	7.373	1.00	102.12
	243	O	LYS	A	367	53.888	57.947	7.915	1.00	103.05

	244	N	GLY	A	368	53.365	59.372	6.265	1.00	99.91
	245	CA	GLY	A	368	52.480	58.388	5.664	1.00	96.70
	246	C	GLY	A	368	51.079	58.800	5.255	1.00	94.03
	247	O	GLY	A	368	50.829	59.949	4.891	1.00	94.76
	248	N	ALA	A	369	50.162	57.839	5.313	1.00	90.44
	249	CA	ALA	A	369	48.772	58.066	4.935	1.00	86.18
	250	CB	ALA	A	369	48.460	57.308	3.645	1.00	86.97
	251	C	ALA	A	369	47.808	57.639	6.038	1.00	82.79
	252	O	ALA	A	369	48.149	56.827	6.897	1.00	83.46
	253	N	VAL	A	370	46.600	58.193	6.001	1.00	78.82
	254	CA	VAL	A	370	45.567	57.881	6.985	1.00	73.44
	255	CB	VAL	A	370	45.161	59.132	7.777	1.00	71.37
	256	CG1	VAL	A	370	44.145	58.763	8.840	1.00	68.72
	257	CG2	VAL	A	370	46.388	59.769	8.404	1.00	66.32
	258	C	VAL	A	370	44.347	57.346	6.252	1.00	71.19
	259	O	VAL	A	370	43.803	58.019	5.383	1.00	70.77
	260	N	ASN	A	371	43.913	56.138	6.605	1.00	69.11
	261	CA	ASN	A	371	42.769	55.531	5.936	1.00	67.35
	262	CB	ASN	A	371	43.145	54.138	5.430	1.00	68.95
	263	CG	ASN	A	371	44.330	54.168	4.498	1.00	73.37
	264	OD1	ASN	A	371	44.299	54.828	3.459	1.00	76.52
	265	ND2	ASN	A	371	45.387	53.454	4.863	1.00	76.06
	266	C	ASN	A	371	41.491	55.441	6.766	1.00	65.35
	267	O	ASN	A	371	41.516	55.146	7.964	1.00	63.63
	268	N	LEU	A	372	40.373	55.708	6.100	1.00	63.51
	269	CA	LEU	A	372	39.060	55.651	6.721	1.00	60.50
	270	CB	LEU	A	372	38.386	57.027	6.705	1.00	60.09
	271	CG	LEU	A	372	39.139	58.170	7.386	1.00	61.37
	272	CD1	LEU	A	372	38.265	59.404	7.412	1.00	63.12
	273	CD2	LEU	A	372	39.517	57.771	8.791	1.00	62.53
	274	C	LEU	A	372	38.220	54.658	5.936	1.00	57.54
	275	O	LEU	A	372	38.069	54.776	4.720	1.00	58.06
	276	N	THR	A	373	37.681	53.674	6.642	1.00	54.64
	277	CA	THR	A	373	36.855	52.648	6.026	1.00	52.59
	278	CB	THR	A	373	37.425	51.254	6.314	1.00	54.37
	279	OG1	THR	A	373	38.799	51.217	5.909	1.00	60.15
	280	CG2	THR	A	373	36.645	50.191	5.555	1.00	57.66
	281	C	THR	A	373	35.444	52.722	6.591	1.00	48.12
	282	O	THR	A	373	35.263	52.797	7.803	1.00	46.78
	283	N	TRP	A	374	34.450	52.705	5.709	1.00	45.42
	284	CA	TRP	A	374	33.057	52.767	6.129	1.00	44.33
	285	CB	TRP	A	374	32.260	53.762	5.277	1.00	40.42
	286	CG	TRP	A	374	32.664	55.183	5.442	1.00	41.22
	287	CD2	TRP	A	374	32.215	56.090	6.457	1.00	35.68
	288	CE2	TRP	A	374	32.841	57.329	6.219	1.00	31.67
	289	CE3	TRP	A	374	31.342	55.972	7.545	1.00	35.08
	290	CD1	TRP	A	374	33.523	55.888	4.652	1.00	38.77
	291	NE1	TRP	A	374	33.634	57.180	5.112	1.00	37.27
	292	CZ2	TRP	A	374	32.621	58.447	7.027	1.00	32.53
	293	CZ3	TRP	A	374	31.121	57.084	8.352	1.00	36.03
	294	CH2	TRP	A	374	31.760	58.304	8.087	1.00	33.34
	295	C	TRP	A	374	32.385	51.405	6.022	1.00	44.84
	296	O	TRP	A	374	32.758	50.581	5.186	1.00	43.54
	297	N	SER	A	375	31.395	51.181	6.882	1.00	44.41
	298	CA	SER	A	375	30.633	49.940	6.887	1.00	45.63
	299	CB	SER	A	375	31.432	48.800	7.535	1.00	47.59
	300	OG	SER	A	375	31.512	48.938	8.943	1.00	49.42
	301	C	SER	A	375	29.308	50.112	7.618	1.00	45.23
	302	O	SER	A	375	29.162	50.991	8.471	1.00	46.27
	303	N	ARG	A	376	28.341	49.277	7.257	1.00	42.63
	304	CA	ARG	A	376	27.033	49.307	7.882	1.00	41.96
	305	CB	ARG	A	376	25.924	49.263	6.834	1.00	43.72

	306	CG	ARG	A	376	25.855	50.458	5.901	1.00	40.62
	307	CD	ARG	A	376	24.405	50.693	5.520	1.00	41.72
	308	NE	ARG	A	376	24.143	50.468	4.110	1.00	52.53
	309	CZ	ARG	A	376	22.929	50.305	3.599	1.00	52.81
	310	NH1	ARG	A	376	21.859	50.335	4.386	1.00	51.46
	311	NH2	ARG	A	376	22.781	50.128	2.293	1.00	56.61
	312	C	ARG	A	376	26.920	48.082	8.775	1.00	39.96
	313	O	ARG	A	376	27.218	46.971	8.355	1.00	40.84
	314	N	ALA	A	377	26.503	48.285	10.014	1.00	41.64
	315	CA	ALA	A	377	26.350	47.177	10.946	1.00	41.34
	316	CB	ALA	A	377	25.705	47.680	12.227	1.00	33.50
	317	C	ALA	A	377	25.502	46.056	10.325	1.00	41.22
	318	O	ALA	A	377	25.685	44.888	10.648	1.00	41.04
	319	N	SER	A	378	24.592	46.421	9.423	1.00	40.92
	320	CA	SER	A	378	23.719	45.451	8.773	1.00	42.71
	321	CB	SER	A	378	22.491	46.139	8.185	1.00	44.29
	322	OG	SER	A	378	22.842	46.867	7.020	1.00	42.78
	323	C	SER	A	378	24.420	44.706	7.658	1.00	43.58
	324	O	SER	A	378	23.851	43.791	7.078	1.00	44.22
	325	N	GLY	A	379	25.646	45.117	7.349	1.00	43.82
	326	CA	GLY	A	379	26.409	44.463	6.304	1.00	45.23
	327	C	GLY	A	379	26.060	44.917	4.901	1.00	48.43
	328	O	GLY	A	379	26.747	44.562	3.943	1.00	47.67
	329	N	LYS	A	380	24.995	45.699	4.763	1.00	50.04
	330	CA	LYS	A	380	24.603	46.177	3.447	1.00	52.22
	331	CB	LYS	A	380	23.238	46.868	3.509	1.00	54.82
	332	CG	LYS	A	380	22.096	45.879	3.646	1.00	63.15
	333	CD	LYS	A	380	20.734	46.528	3.466	1.00	70.67
	334	CE	LYS	A	380	19.640	45.467	3.455	1.00	75.50
	335	NZ	LYS	A	380	18.275	46.051	3.354	1.00	80.58
	336	C	LYS	A	380	25.655	47.107	2.851	1.00	52.26
	337	O	LYS	A	380	26.495	47.656	3.565	1.00	49.96
	338	N	PRO	A	381	25.626	47.285	1.522	1.00	53.55
	339	CD	PRO	A	381	24.694	46.657	0.571	1.00	54.43
	340	CA	PRO	A	381	26.584	48.147	0.818	1.00	54.97
	341	CB	PRO	A	381	26.212	47.948	-0.655	1.00	57.06
	342	CG	PRO	A	381	25.519	46.611	-0.673	1.00	59.10
	343	C	PRO	A	381	26.532	49.626	1.207	1.00	54.14
	344	O	PRO	A	381	25.457	50.178	1.467	1.00	55.04
	345	N	VAL	A	382	27.701	50.256	1.251	1.00	52.78
	346	CA	VAL	A	382	27.801	51.680	1.546	1.00	53.97
	347	CB	VAL	A	382	28.891	51.997	2.611	1.00	54.50
	348	CG1	VAL	A	382	28.595	51.252	3.896	1.00	56.74
	349	CG2	VAL	A	382	30.281	51.645	2.078	1.00	46.72
	350	C	VAL	A	382	28.202	52.338	0.226	1.00	54.10
	351	O	VAL	A	382	28.910	51.735	-0.583	1.00	53.38
	352	N	ASN	A	383	27.752	53.566	0.011	1.00	53.55
	353	CA	ASN	A	383	28.073	54.289	-1.210	1.00	54.35
	354	CB	ASN	A	383	27.135	55.485	-1.370	1.00	60.43
	355	CG	ASN	A	383	25.677	55.087	-1.371	1.00	67.43
	356	OD1	ASN	A	383	24.806	55.890	-1.037	1.00	75.26
	357	ND2	ASN	A	383	25.399	53.845	-1.756	1.00	72.99
	358	C	ASN	A	383	29.520	54.779	-1.218	1.00	52.64
	359	O	ASN	A	383	30.292	54.518	-0.293	1.00	50.26
	360	N	HIS	A	384	29.879	55.493	-2.276	1.00	51.74
	361	CA	HIS	A	384	31.225	56.038	-2.415	1.00	51.28
	362	CB	HIS	A	384	31.499	56.380	-3.879	1.00	59.06
	363	CG	HIS	A	384	31.657	55.179	-4.761	1.00	65.42
	364	CD2	HIS	A	384	30.912	54.727	-5.796	1.00	72.26
	365	ND1	HIS	A	384	32.694	54.284	-4.615	1.00	70.87
	366	CE1	HIS	A	384	32.581	53.330	-5.523	1.00	76.58
	367	NE2	HIS	A	384	31.507	53.576	-6.253	1.00	77.95

	368	C	HIS	A	384	31.362	57.294	-1.555	1.00	47.99
	369	O	HIS	A	384	30.478	56.145	-1.544	1.00	45.37
	370	N	SER	A	385	32.473	57.413	-0.844	1.00	45.57
	371	CA	SER	A	385	32.674	58.564	0.015	1.00	45.69
	372	CB	SER	A	385	33.134	58.097	1.405	1.00	41.19
	373	OG	SER	A	385	34.299	57.285	1.338	1.00	41.34
	374	C	SER	A	385	33.654	59.598	-0.560	1.00	44.94
	375	O	SER	A	385	34.413	59.313	-1.482	1.00	41.64
	376	N	THR	A	386	33.603	60.805	-0.007	1.00	45.73
	377	CA	THR	A	386	34.467	61.898	-0.421	1.00	46.08
	378	CB	THR	A	386	33.670	63.191	-0.637	1.00	47.42
	379	OG1	THR	A	386	32.775	63.024	-1.744	1.00	50.45
	380	CG2	THR	A	386	34.615	64.347	-0.925	1.00	51.73
	381	C	THR	A	386	35.487	62.132	0.681	1.00	46.45
	382	O	THR	A	386	35.129	62.241	1.853	1.00	47.06
	383	N	ARG	A	387	36.754	62.206	0.292	1.00	46.33
	384	CA	ARG	A	387	37.849	62.410	1.228	1.00	46.50
	385	CB	ARG	A	387	38.874	61.290	1.030	1.00	48.08
	386	CG	ARG	A	387	40.086	61.366	1.933	1.00	54.89
	387	CD	ARG	A	387	41.208	60.481	1.405	1.00	59.67
	388	NE	ARG	A	387	42.438	60.668	2.165	1.00	63.12
	389	CZ	ARG	A	387	42.775	59.950	3.230	1.00	65.65
	390	NH1	ARG	A	387	41.971	58.982	3.651	1.00	67.29
	391	NH2	ARG	A	387	43.899	60.215	3.889	1.00	63.40
	392	C	ARG	A	387	38.517	63.786	1.046	1.00	46.30
	393	O	ARG	A	387	38.733	64.239	-0.079	1.00	44.30
	394	N	LYS	A	388	38.834	64.441	2.162	1.00	45.70
	395	CA	LYS	A	388	39.489	65.749	2.140	1.00	44.68
	396	CB	LYS	A	388	38.479	66.852	2.466	1.00	46.84
	397	CG	LYS	A	388	37.337	66.931	1.476	1.00	56.94
	398	CD	LYS	A	388	36.150	67.679	2.054	1.00	58.62
	399	CE	LYS	A	388	34.883	67.307	1.309	1.00	61.92
	400	NZ	LYS	A	388	33.676	67.856	1.977	1.00	70.07
	401	C	LYS	A	388	40.646	65.798	3.143	1.00	44.52
	402	O	LYS	A	388	40.502	65.379	4.294	1.00	40.60
	403	N	GLU	A	389	41.793	66.304	2.689	1.00	47.26
	404	CA	GLU	A	389	43.001	66.424	3.518	1.00	50.72
	405	CB	GLU	A	389	44.114	65.531	2.965	1.00	54.88
	406	CG	GLU	A	389	43.848	64.041	3.039	1.00	67.37
	407	CD	GLU	A	389	44.979	63.225	2.436	1.00	75.83
	408	OE1	GLU	A	389	46.116	63.742	2.364	1.00	79.33
	409	OE2	GLU	A	389	44.738	62.062	2.044	1.00	80.70
	410	C	GLU	A	389	43.510	67.871	3.551	1.00	51.11
	411	O	GLU	A	389	43.644	68.510	2.504	1.00	48.28
	412	N	ALA	A	390	43.814	68.382	4.741	1.00	52.07
	413	CA	ALA	A	390	44.297	69.755	4.868	1.00	56.84
	414	CB	ALA	A	390	43.120	70.712	4.972	1.00	53.86
	415	C	ALA	A	390	45.229	69.957	6.058	1.00	60.96
	416	O	ALA	A	390	45.085	69.315	7.098	1.00	61.14
	417	N	ALA	A	391	46.179	70.873	5.896	1.00	65.61
	418	CA	ALA	A	391	47.151	71.187	6.938	1.00	68.46
	419	CB	ALA	A	391	48.398	70.336	6.761	1.00	71.73
	420	C	ALA	A	391	47.518	72.661	6.866	1.00	70.37
	421	O	ALA	A	391	47.076	73.461	7.688	1.00	72.17
	422	N	LEU	A	397	47.315	68.210	11.080	1.00	60.70
	423	CA	LEU	A	397	46.686	67.651	9.890	1.00	61.36
	424	CB	LEU	A	397	47.489	66.458	9.375	1.00	64.28
	425	CG	LEU	A	397	46.854	65.736	8.180	1.00	65.19
	426	CD1	LEU	A	397	46.802	66.670	6.981	1.00	65.40
	427	CD2	LEU	A	397	47.652	64.485	7.844	1.00	68.57
	428	C	LEU	A	397	45.241	67.211	10.119	1.00	61.24
	429	O	LEU	A	397	44.934	66.485	11.064	1.00	62.11

	430	N	THR	A	398	44.360	67.654	9.233	1.00	59.83
	431	CA	THR	A	398	42.950	67.309	9.305	1.00	58.04
	432	CB	THR	A	398	42.061	68.572	9.263	1.00	58.72
	433	OG1	THR	A	398	42.171	69.278	10.506	1.00	64.28
	434	CG2	THR	A	398	40.608	68.197	9.023	1.00	61.55
	435	C	THR	A	398	42.573	66.401	8.135	1.00	55.72
	436	O	THR	A	398	43.021	66.595	7.000	1.00	55.02
	437	N	VAL	A	399	41.752	65.401	8.422	1.00	52.38
	438	CA	VAL	A	399	41.297	64.473	7.402	1.00	49.13
	439	CB	VAL	A	399	42.143	63.179	7.391	1.00	51.57
	440	CG1	VAL	A	399	41.594	62.212	6.363	1.00	52.00
	441	CG2	VAL	A	399	43.590	63.500	7.068	1.00	55.81
	442	C	VAL	A	399	39.847	64.093	7.643	1.00	46.27
	443	O	VAL	A	399	39.478	63.649	8.732	1.00	43.17
	444	N	THR	A	400	39.015	64.289	6.630	1.00	44.56
	445	CA	THR	A	400	37.619	63.915	6.758	1.00	43.39
	446	CB	THR	A	400	36.669	65.140	6.829	1.00	41.43
	447	OG1	THR	A	400	36.628	65.794	5.557	1.00	48.65
	448	CG2	THR	A	400	37.126	66.120	7.889	1.00	38.93
	449	C	THR	A	400	37.174	63.059	5.584	1.00	40.85
	450	O	THR	A	400	37.751	63.094	4.494	1.00	35.85
	451	N	SER	A	401	36.146	62.267	5.847	1.00	39.13
	452	CA	SER	A	401	35.542	61.417	4.847	1.00	37.93
	453	CB	SER	A	401	35.885	59.944	5.079	1.00	40.15
	454	OG	SER	A	401	35.290	59.142	4.069	1.00	44.51
	455	C	SER	A	401	34.054	61.622	5.044	1.00	36.16
	456	O	SER	A	401	33.552	61.461	6.153	1.00	36.19
	457	N	THR	A	402	33.362	61.989	3.975	1.00	32.94
	458	CA	THR	A	402	31.931	62.204	4.039	1.00	32.35
	459	CB	THR	A	402	31.578	63.578	3.483	1.00	33.13
	460	OG1	THR	A	402	32.279	64.559	4.246	1.00	34.46
	461	CG2	THR	A	402	30.086	63.845	3.577	1.00	33.71
	462	C	THR	A	402	31.222	61.117	3.243	1.00	31.66
	463	O	THR	A	402	31.512	60.886	2.064	1.00	26.99
	464	N	LEU	A	403	30.282	60.459	3.913	1.00	32.16
	465	CA	LEU	A	403	29.526	59.370	3.319	1.00	32.46
	466	CB	LEU	A	403	29.648	58.123	4.205	1.00	34.12
	467	CG	LEU	A	403	28.920	56.838	3.794	1.00	34.78
	468	CD1	LEU	A	403	29.678	56.196	2.644	1.00	35.87
	469	CD2	LEU	A	403	28.856	55.873	4.968	1.00	31.42
	470	C	LEU	A	403	28.052	59.690	3.099	1.00	33.39
	471	O	LEU	A	403	27.321	60.005	4.040	1.00	30.14
	472	N	PRO	A	404	27.604	59.633	1.835	1.00	34.13
	473	CD	PRO	A	404	28.391	59.413	0.605	1.00	34.29
	474	CA	PRO	A	404	26.203	59.899	1.513	1.00	34.91
	475	CB	PRO	A	404	26.161	59.777	-0.008	1.00	33.92
	476	CG	PRO	A	404	27.554	60.121	-0.426	1.00	33.77
	477	C	PRO	A	404	25.427	58.773	2.191	1.00	36.43
	478	O	PRO	A	404	25.824	57.610	2.140	1.00	30.87
	479	N	VAL	A	405	24.326	59.120	2.835	1.00	37.52
	480	CA	VAL	A	405	23.532	58.129	3.531	1.00	41.37
	481	CB	VAL	A	405	23.522	58.462	5.053	1.00	44.39
	482	CG1	VAL	A	405	22.100	58.566	5.587	1.00	47.81
	483	CG2	VAL	A	405	24.312	57.420	5.799	1.00	43.63
	484	C	VAL	A	405	22.108	58.056	2.980	1.00	42.93
	485	O	VAL	A	405	21.558	59.047	2.511	1.00	42.10
	486	N	GLY	A	406	21.518	56.868	3.019	1.00	45.32
	487	CA	GLY	A	406	20.154	56.731	2.547	1.00	46.40
	488	C	GLY	A	406	19.227	57.392	3.552	1.00	46.70
	489	O	GLY	A	406	19.421	57.255	4.766	1.00	41.89
	490	N	THR	A	407	18.227	58.114	3.048	1.00	46.37
	491	CA	THR	A	407	17.259	58.809	3.892	1.00	49.05

55	492	CB	THR	A	407	16.252	59.617	3.038	1.00	51.01
	493	OG1	THR	A	407	16.929	60.700	2.391	1.00	55.76
	494	CG2	THR	A	407	15.147	60.177	3.905	1.00	54.66
	495	C	THR	A	407	16.468	57.854	4.775	1.00	49.24
	496	O	THR	A	407	16.446	58.003	5.995	1.00	48.91
5	497	N	ALA	A	408	15.823	56.874	4.147	1.00	49.71
	498	CA	ALA	A	408	15.008	55.907	4.860	1.00	50.13
	499	CB	ALA	A	408	14.233	55.038	3.876	1.00	53.74
	500	C	ALA	A	408	15.823	55.031	5.788	1.00	51.25
	501	O	ALA	A	408	15.393	54.748	6.909	1.00	50.28
10	502	N	ASP	A	409	16.995	54.600	5.330	1.00	50.74
	503	CA	ASP	A	409	17.852	53.748	6.152	1.00	52.13
	504	CB	ASP	A	409	19.102	53.335	5.370	1.00	58.27
	505	CG	ASP	A	409	18.770	52.535	4.123	1.00	69.38
	506	OD1	ASP	A	409	18.105	51.479	4.252	1.00	75.94
15	507	OD2	ASP	A	409	19.169	52.959	3.016	1.00	72.00
	508	C	ASP	A	409	18.259	54.449	7.445	1.00	49.96
	509	O	ASP	A	409	18.317	53.831	8.512	1.00	49.48
	510	N	TRP	A	410	18.542	55.742	7.345	1.00	46.74
	511	CA	TRP	A	410	18.931	56.494	8.517	1.00	44.75
20	512	CB	TRP	A	410	19.487	57.868	8.143	1.00	39.75
	513	CG	TRP	A	410	19.913	58.601	9.362	1.00	37.35
	514	CD2	TRP	A	410	21.131	58.409	10.083	1.00	31.03
	515	CE2	TRP	A	410	21.049	59.188	11.254	1.00	29.68
	516	CE3	TRP	A	410	22.286	57.637	9.857	1.00	32.46
25	517	CD1	TRP	A	410	19.166	59.481	10.099	1.00	32.61
	518	NE1	TRP	A	410	19.842	59.833	11.232	1.00	33.45
	519	CZ2	TRP	A	410	22.078	59.230	12.200	1.00	29.11
	520	CZ3	TRP	A	410	23.310	57.680	10.798	1.00	34.12
	521	CH2	TRP	A	410	23.195	58.472	11.958	1.00	35.80
30	522	C	TRP	A	410	17.743	56.666	9.451	1.00	43.08
	523	O	TRP	A	410	17.867	56.463	10.655	1.00	38.95
	524	N	ILE	A	411	16.593	57.037	8.894	1.00	46.39
	525	CA	ILE	A	411	15.389	57.228	9.696	1.00	51.22
	526	CB	ILE	A	411	14.218	57.752	8.841	1.00	53.02
35	527	CG2	ILE	A	411	12.972	57.895	9.699	1.00	55.27
	528	CG1	ILE	A	411	14.590	59.112	8.240	1.00	56.63
	529	CD1	ILE	A	411	13.498	59.742	7.367	1.00	61.16
	530	C	ILE	A	411	14.968	55.931	10.371	1.00	52.33
	531	O	ILE	A	411	14.404	55.955	11.462	1.00	53.32
40	532	N	GLU	A	412	15.267	54.800	9.731	1.00	54.18
	533	CA	GLU	A	412	14.907	53.501	10.279	1.00	53.56
	534	CB	GLU	A	412	14.692	52.490	9.158	1.00	58.95
	535	CG	GLU	A	412	13.298	52.566	8.572	1.00	73.61
	536	CD	GLU	A	412	13.058	51.538	7.488	1.00	83.01
45	537	OE1	GLU	A	412	13.415	50.356	7.689	1.00	89.18
	538	OE2	GLU	A	412	12.498	51.909	6.435	1.00	89.24
	539	C	GLU	A	412	15.874	52.935	11.307	1.00	51.42
	540	O	GLU	A	412	15.615	51.875	11.873	1.00	50.68
	541	N	GLY	A	413	16.983	53.633	11.549	1.00	48.27
50	542	CA	GLY	A	413	17.929	53.172	12.549	1.00	46.15
	543	C	GLY	A	413	19.223	52.489	12.133	1.00	44.58
	544	O	GLY	A	413	19.925	51.963	12.994	1.00	42.91
	545	N	GLU	A	414	19.556	52.482	10.844	1.00	44.06
	546	CA	GLU	A	414	20.801	51.851	10.415	1.00	42.21
55	547	CB	GLU	A	414	21.077	52.133	8.928	1.00	42.27
	548	CG	GLU	A	414	22.441	51.637	8.402	1.00	44.30
	549	CD	GLU	A	414	22.564	50.113	8.361	1.00	52.18

	550	OE1	GLU	A	414	23.038	49.517	9.355	1.00	51.39
	551	OE2	GLU	A	414	22.175	49.510	7.336	1.00	49.53
	552	C	GLU	A	414	21.910	52.453	11.261	1.00	41.40
	553	O	GLU	A	414	21.819	53.605	11.687	1.00	38.41
	554	N	THR	A	415	22.944	51.664	11.527	1.00	41.90
	555	CA	THR	A	415	24.078	52.146	12.294	1.00	43.26
	556	CB	THR	A	415	24.259	51.319	13.594	1.00	46.09
	557	OG1	THR	A	415	25.604	51.445	14.068	1.00	50.78
	558	CG2	THR	A	415	23.910	49.884	13.366	1.00	56.55
	559	C	THR	A	415	25.330	52.101	11.410	1.00	41.87
	560	O	THR	A	415	25.637	51.067	10.815	1.00	43.61
	561	N	TYR	A	416	26.029	53.229	11.294	1.00	39.27
	562	CA	TYR	A	416	27.222	53.291	10.450	1.00	37.37
	563	CB	TYR	A	416	27.172	54.498	9.519	1.00	33.61
	564	CG	TYR	A	416	25.967	54.536	8.622	1.00	27.57
	565	CD1	TYR	A	416	24.706	54.847	9.126	1.00	26.31
	566	CE1	TYR	A	416	23.591	54.848	8.300	1.00	35.08
	567	CD2	TYR	A	416	26.084	54.229	7.275	1.00	28.68
	568	CE2	TYR	A	416	24.985	54.221	6.449	1.00	30.56
	569	CZ	TYR	A	416	23.743	54.530	6.960	1.00	35.62
	570	OH	TYR	A	416	22.656	54.512	6.116	1.00	44.94
	571	C	TYR	A	416	28.494	53.344	11.267	1.00	38.31
	572	O	TYR	A	416	28.508	53.856	12.391	1.00	37.29
	573	N	GLN	A	417	29.569	52.819	10.684	1.00	39.74
	574	CA	GLN	A	417	30.849	52.777	11.364	1.00	40.75
	575	CB	GLN	A	417	31.143	51.346	11.836	1.00	41.60
	576	CG	GLN	A	417	32.360	51.247	12.751	1.00	53.57
	577	CD	GLN	A	417	32.603	49.838	13.271	1.00	65.04
	578	OE1	GLN	A	417	33.476	49.119	12.775	1.00	69.74
	579	NE2	GLN	A	417	31.823	49.435	14.269	1.00	66.91
	580	C	GLN	A	417	32.022	53.280	10.535	1.00	39.48
	581	O	GLN	A	417	32.149	52.981	9.346	1.00	40.03
	582	N	CYS	A	418	32.882	54.043	11.188	1.00	39.47
	583	CA	CYS	A	418	34.075	54.568	10.559	1.00	41.39
	584	C	CYS	A	418	35.246	53.868	11.232	1.00	41.00
	585	O	CYS	A	418	35.395	53.939	12.452	1.00	41.94
	586	CB	CYS	A	418	34.187	56.087	10.781	1.00	39.12
	587	SG	CYS	A	418	35.688	56.818	10.050	1.00	53.87
	588	N	ALA	A	419	36.059	53.171	10.446	1.00	42.75
	589	CA	ALA	A	419	37.238	52.498	10.982	1.00	45.21
	590	CB	ALA	A	419	37.357	51.073	10.412	1.00	45.00
	591	C	ALA	A	419	38.462	53.335	10.602	1.00	46.28
	592	O	ALA	A	419	38.826	53.428	9.429	1.00	44.60
	593	N	VAL	A	420	39.088	53.961	11.592	1.00	49.65
	594	CA	VAL	A	420	40.252	54.789	11.322	1.00	54.91
	595	CB	VAL	A	420	40.295	56.016	12.245	1.00	52.57
	596	CG1	VAL	A	420	41.515	56.858	11.911	1.00	54.41
	597	CG2	VAL	A	420	39.032	56.844	12.083	1.00	52.89
	598	C	VAL	A	420	41.564	54.028	11.477	1.00	59.75
	599	O	VAL	A	420	41.877	53.517	12.556	1.00	56.32
	600	N	THR	A	421	42.325	53.960	10.387	1.00	65.72
	601	CA	THR	A	421	43.615	53.278	10.383	1.00	72.95
	602	CB	THR	A	421	43.733	52.297	9.197	1.00	73.73
	603	OG1	THR	A	421	42.702	51.306	9.282	1.00	78.26
	604	CG2	THR	A	421	45.082	51.605	9.217	1.00	74.84
	605	C	THR	A	421	44.741	54.298	10.269	1.00	76.77
	606	O	THR	A	421	45.141	54.663	9.164	1.00	76.76
	607	N	ALA	A	422	45.248	54.757	11.410	1.00	81.68
	608	CA	ALA	A	422	46.330	55.738	11.427	1.00	86.81
	609	CB	ALA	A	422	46.358	56.466	12.768	1.00	86.67
	610	C	ALA	A	422	47.670	55.060	11.178	1.00	90.55
	611	O	ALA	A	422	47.843	53.876	11.477	1.00	91.00

	612	N	PRO	A	423	48.641	55.807	10.625	1.00	93.77
	613	CD	PRO	A	423	48.615	57.260	10.385	1.00	94.85
	614	CA	PRO	A	423	49.970	55.257	10.341	1.00	95.83
	615	CB	PRO	A	423	50.731	56.459	9.791	1.00	96.70
	616	CG	PRO	A	423	50.074	57.619	10.487	1.00	97.10
	617	C	PRO	A	423	50.612	54.674	11.596	1.00	97.16
	618	O	PRO	A	423	50.850	53.472	11.674	1.00	97.34
	619	N	ALA	A	424	50.893	55.524	12.578	1.00	98.50
	620	CA	ALA	A	424	51.486	55.063	13.829	1.00	99.73
	621	CB	ALA	A	424	51.995	56.252	14.626	1.00	99.11
	622	C	ALA	A	424	50.412	54.318	14.625	1.00	100.69
	623	O	ALA	A	424	49.503	53.725	14.046	1.00	101.64
	624	N	LEU	A	425	50.521	54.355	15.950	1.00	100.65
	625	CA	LEU	A	425	49.550	53.705	16.828	1.00	99.91
	626	CB	LEU	A	425	48.182	54.372	16.671	1.00	100.27
	627	CG	LEU	A	425	48.126	55.833	17.125	1.00	102.88
	628	CD1	LEU	A	425	46.735	56.386	16.889	1.00	102.68
	629	CD2	LEU	A	425	48.498	55.932	18.603	1.00	105.00
	630	C	LEU	A	425	49.427	52.200	16.586	1.00	98.82
	631	O	LEU	A	425	49.985	51.676	15.629	1.00	98.87
	632	N	PRO	A	426	48.712	51.485	17.475	1.00	97.69
	633	CD	PRO	A	426	48.418	51.939	18.849	1.00	98.02
	634	CA	PRO	A	426	48.513	50.034	17.361	1.00	95.83
	635	CB	PRO	A	426	48.673	49.570	18.797	1.00	96.48
	636	CG	PRO	A	426	47.965	50.659	19.545	1.00	96.97
	637	C	PRO	A	426	47.145	49.651	16.791	1.00	94.21
	638	O	PRO	A	426	47.006	49.360	15.602	1.00	94.03
	639	N	ARG	A	427	46.140	49.637	17.661	1.00	92.33
	640	CA	ARG	A	427	44.778	49.297	17.269	1.00	90.72
	641	CB	ARG	A	427	43.928	49.017	18.510	1.00	92.36
	642	CG	ARG	A	427	44.349	47.816	19.342	1.00	96.36
	643	CD	ARG	A	427	43.525	46.585	18.998	1.00	99.46
	644	NE	ARG	A	427	43.247	45.778	20.184	1.00	101.30
	645	CZ	ARG	A	427	42.540	46.203	21.228	1.00	102.28
	646	NH1	ARG	A	427	42.037	47.430	21.236	1.00	102.89
	647	NH2	ARG	A	427	42.334	45.400	22.264	1.00	102.96
	648	C	ARG	A	427	44.152	50.458	16.505	1.00	88.67
	649	O	ARG	A	427	44.292	51.614	16.902	1.00	88.90
	650	N	ALA	A	428	43.462	50.153	15.413	1.00	85.79
	651	CA	ALA	A	428	42.807	51.188	14.631	1.00	82.45
	652	CB	ALA	A	428	42.310	50.615	13.311	1.00	82.49
	653	C	ALA	A	428	41.637	51.707	15.456	1.00	79.74
	654	O	ALA	A	428	41.032	50.955	16.221	1.00	79.87
	655	N	LEU	A	429	41.330	52.994	15.315	1.00	76.91
	656	CA	LEU	A	429	40.223	53.604	16.049	1.00	72.60
	657	CB	LEU	A	429	40.405	55.125	16.126	1.00	73.30
	658	CG	LEU	A	429	41 684	55.685	16.757	1.00	75.14
	659	CD1	LEU	A	429	41.706	57.197	16.600	1.00	70.88
	660	CD2	LEU	A	429	41.756	55.296	18.227	1.00	79.00
	661	C	LEU	A	429	38.921	53.290	15.323	1.00	69.58
	662	O	LEU	A	429	38.894	53.209	14.094	1.00	67.68
	663	N	MET	A	430	37.845	53.116	16.085	1.00	66.58
	664	CA	MET	A	430	36.543	52.815	15.504	1.00	63.72
	665	CB	MET	A	430	36.203	51.340	15.704	1.00	66.69
	666	CG	MET	A	430	37.237	50.395	15.125	1.00	76.81
	667	SD	MET	A	430	36.764	48.668	15.345	1.00	89.36
	668	CE	MET	A	430	36.990	48.471	17.110	1.00	87.45
	669	C	MET	A	430	35.450	53.674	16.119	1.00	59.15
	670	O	MET	A	430	35.371	53.822	17.340	1.00	59.09
	671	N	ARG	A	431	34.607	54.245	15.267	1.00	55.24
	672	CA	ARG	A	431	33.523	55.091	15.746	1.00	51.07
	673	CB	ARG	A	431	33.863	56.564	15.516	1.00	51.17

	674	CG	ARG	A	431	35.291	56.939	15.897	1.00	55.59
	675	CD	ARG	A	431	35.320	58.159	16.805	1.00	67.55
	676	NE	ARG	A	431	35.147	57.816	18.216	1.00	74.62
	677	CZ	ARG	A	431	36.128	57.380	19.001	1.00	76.90
	678	NH1	ARG	A	431	37.353	57.236	18.514	1.00	77.02
	679	NH2	ARG	A	431	35.888	57.087	20.274	1.00	79.64
	680	C	ARG	A	431	32.244	54.732	15.013	1.00	47.90
	681	O	ARG	A	431	32.277	54.386	13.832	1.00	46.26
	682	N	SER	A	432	31.120	54.812	15.715	1.00	45.54
	683	CA	SER	A	432	29.832	54.495	15.112	1.00	45.94
	684	CB	SER	A	432	29.356	53.116	15.584	1.00	47.12
	685	OG	SER	A	432	29.331	53.040	16.994	1.00	50.92
	686	C	SER	A	432	28.764	55.537	15.412	1.00	43.27
	687	O	SER	A	432	28.862	56.272	16.391	1.00	42.70
	688	N	THR	A	433	27.736	55.588	14.569	1.00	40.97
	689	CA	THR	A	433	26.663	56.552	14.758	1.00	38.90
	690	CB	THR	A	433	26.967	57.875	14.027	1.00	39.50
	691	OG1	THR	A	433	25.911	58.808	14.280	1.00	38.91
	692	CG2	THR	A	433	27.093	57.646	12.516	1.00	36.51
	693	C	THR	A	433	25.329	56.017	14.262	1.00	39.62
	694	O	THR	A	433	25.283	55.188	13.356	1.00	39.87
	695	N	THR	A	434	24.249	56.495	14.876	1.00	39.10
	696	CA	THR	A	434	22.889	56.101	14.531	1.00	39.67
	697	CB	THR	A	434	22.480	54.812	15.282	1.00	43.40
	698	OG1	THR	A	434	22.307	55.104	16.675	1.00	53.59
	699	CG2	THR	A	434	23.559	53.770	15.171	1.00	52.29
	700	C	THR	A	434	21.939	57.220	14.969	1.00	38.41
	701	O	THR	A	434	22.325	58.110	15.726	1.00	38.84
	702	N	ALA	A	435	20.701	57.179	14.506	1.00	37.73
	703	CA	ALA	A	435	19.747	58.190	14.911	1.00	44.38
	704	CB	ALA	A	435	18.426	57.968	14.213	1.00	40.72
	705	C	ALA	A	435	19.577	58.033	16.421	1.00	47.78
	706	O	ALA	A	435	19.611	56.919	16.937	1.00	46.98
	707	N	THR	A	436	19.413	59.146	17.129	1.00	52.31
	708	CA	THR	A	436	19.217	59.094	18.574	1.00	55.83
	709	CB	THR	A	436	19.492	60.469	19.240	1.00	59.83
	710	OG1	THR	A	436	20.873	60.816	19.072	1.00	62.64
	711	CG2	THR	A	436	19.159	60.425	20.732	1.00	60.56
	712	C	THR	A	436	17.766	58.707	18.840	1.00	56.91
	713	O	THR	A	436	16.852	59.242	18.212	1.00	55.51
	714	N	SER	A	437	17.557	57.759	19.748	1.00	58.87
	715	CA	SER	A	437	16.202	57.344	20.095	1.00	61.80
	716	CB	SER	A	437	16.155	55.854	20.474	1.00	63.69
	717	OG	SER	A	437	16.984	55.571	21.589	1.00	67.24
	718	C	SER	A	437	15.753	58.203	21.272	1.00	61.35
	719	O	SER	A	437	16.477	59.111	21.690	1.00	61.92
	720	N	GLY	A	438	14.567	57.930	21.803	1.00	60.43
	721	CA	GLY	A	438	14.087	58.719	22.923	1.00	59.27
	722	C	GLY	A	438	12.999	59.691	22.510	1.00	58.25
	723	O	GLY	A	438	12.739	59.847	21.321	1.00	58.13
	724	N	PRO	A	439	12.347	60.363	23.472	1.00	58.84
	725	CD	PRO	A	439	12.555	60.215	24.923	1.00	60.09
	726	CA	PRO	A	439	11.275	61.323	23.203	1.00	57.04
	727	CB	PRO	A	439	10.908	61.832	24.597	1.00	57.59
	728	CG	PRO	A	439	11.224	60.667	25.472	1.00	59.40
	729	C	PRO	A	439	11.691	62.453	22.272	1.00	54.66
	730	O	PRO	A	439	12.877	62.776	22.155	1.00	56.08
	731	N	ARG	A	440	10.703	63.052	21.618	1.00	51.95
	732	CA	ARG	A	440	10.942	64.149	20.695	1.00	49.50
	733	CB	ARG	A	440	10.471	63.771	19.283	1.00	51.89
	734	CG	ARG	A	440	10.921	62.400	18.791	1.00	59.84
	735	CD	ARG	A	440	12.412	62.334	18.465	1.00	66.22

	736	NE	ARG	A	440	12.845	60.943	18.313	1.00	74.61
	737	CZ	ARG	A	440	14.047	60.555	17.896	1.00	76.10
	738	NH1	ARG	A	440	14.967	61.444	17.573	1.00	77.20
	739	NH2	ARG	A	440	14.328	59.262	17.805	1.00	84.96
	740	C	ARG	A	440	10.145	65.351	21.190	1.00	46.80
	741	O	ARG	A	440	9.058	65.194	21.746	1.00	46.09
	742	N	ALA	A	441	10.696	66.547	21.001	1.00	42.67
	743	CA	ALA	A	441	10.024	67.779	21.402	1.00	39.13
	744	CB	ALA	A	441	10.384	68.142	22.837	1.00	32.25
	745	C	ALA	A	441	10.452	68.888	20.454	1.00	39.00
	746	O	ALA	A	441	11.639	69.045	20.175	1.00	38.16
	747	N	ALA	A	442	9.482	69.651	19.964	1.00	37.20
	748	CA	ALA	A	442	9.736	70.739	19.037	1.00	37.26
	749	CB	ALA	A	442	8.413	71.288	18.526	1.00	37.47
	750	C	ALA	A	442	10.568	71.882	19.617	1.00	39.85
	751	O	ALA	A	442	10.612	72.090	20.825	1.00	41.57
	752	N	PRO	A	443	11.246	72.640	18.743	1.00	39.83
	753	CD	PRO	A	443	11.478	72.297	17.334	1.00	40.96
	754	CA	PRO	A	443	12.080	73.775	19.131	1.00	38.29
	755	CB	PRO	A	443	13.058	73.922	17.956	1.00	36.98
	756	CG	PRO	A	443	12.907	72.675	17.168	1.00	36.14
	757	C	PRO	A	443	11.220	75.037	19.272	1.00	40.19
	758	O	PRO	A	443	10.204	75.194	18.588	1.00	40.51
	759	N	ALA	A	444	11.636	75.927	20.163	1.00	39.07
	760	CA	ALA	A	444	10.942	77.188	20.376	1.00	36.58
	761	CB	ALA	A	444	10.605	77.372	21.860	1.00	40.22
	762	C	ALA	A	444	11.962	78.227	19.919	1.00	34.33
	763	O	ALA	A	444	13.109	78.242	20.398	1.00	30.65
	764	N	VAL	A	445	11.543	79.081	18.991	1.00	28.37
	765	CA	VAL	A	445	12.428	80.080	18.436	1.00	26.39
	766	CB	VAL	A	445	12.448	79.948	16.902	1.00	26.69
	767	CG1	VAL	A	445	13.395	80.980	16.310	1.00	23.97
	768	CG2	VAL	A	445	12.853	78.524	16.514	1.00	22.56
	769	C	VAL	A	445	12.103	81.532	18.809	1.00	27.26
	770	O	VAL	A	445	10.956	81.954	18.733	1.00	24.12
	771	N	TYR	A	446	13.127	82.281	19.207	1.00	23.45
	772	CA	TYR	A	446	12.955	83.681	19.559	1.00	25.54
	773	CB	TYR	A	446	12.868	83.878	21.085	1.00	24.97
	774	CG	TYR	A	446	12.704	85.336	21.440	1.00	24.95
	775	CD1	TYR	A	446	11.639	86.083	20.918	1.00	37.39
	776	CE1	TYR	A	446	11.506	87.454	21.193	1.00	34.09
	777	CD2	TYR	A	446	13.627	85.987	22.249	1.00	28.20
	778	CE2	TYR	A	446	13.508	87.355	22.533	1.00	31.02
	779	CZ	TYR	A	446	12.440	88.081	21.998	1.00	34.30
	780	OH	TYR	A	446	12.306	89.426	22.254	1.00	35.42
	781	C	TYR	A	446	14.135	84.470	19.012	1.00	23.87
	782	O	TYR	A	446	15.275	84.279	19.437	1.00	28.38
	783	N	ALA	A	447	13.858	85.346	18.058	1.00	26.40
	784	CA	ALA	A	447	14.893	86.155	17.429	1.00	27.30
	785	CB	ALA	A	447	14.766	86.065	15.905	1.00	24.55
	786	C	ALA	A	447	14.760	87.598	17.898	1.00	30.87
	787	O	ALA	A	447	13.655	88.085	18.121	1.00	32.42
	788	N	PHE	A	448	15.880	88.290	18.055	1.00	31.33
	789	CA	PHE	A	448	15.801	89.661	18.518	1.00	34.25
	790	CB	PHE	A	448	15.616	89.662	20.040	1.00	40.48
	791	CG	PHE	A	448	16.795	89.103	20.786	1.00	39.26
	792	CD1	PHE	A	448	17.837	89.937	21.177	1.00	39.27
	793	CD2	PHE	A	448	16.896	87.738	21.041	1.00	36.97
	794	CE1	PHE	A	448	18.967	89.420	21.814	1.00	43.41
	795	CE2	PHE	A	448	18.022	87.211	21.678	1.00	36.78
	796	CZ	PHE	A	448	19.059	88.054	22.064	1.00	37.14
	797	C	PHE	A	448	17.021	90.487	18.148	1.00	34.75

	798	O	PHE	A	448	18.046	89.954	17.731	1.00	34.97
	799	N	ALA	A	449	16.892	91.799	18.302	1.00	37.02
	800	CA	ALA	A	449	17.977	92.723	18.021	1.00	38.65
	801	CB	ALA	A	449	17.478	93.869	17.202	1.00	32.34
	802	C	ALA	A	449	18.550	93.250	19.333	1.00	42.92
	803	O	ALA	A	449	17.826	93.435	20.306	1.00	42.07
	804	N	THR	A	450	19.857	93.489	19.341	1.00	47.71
	805	CA	THR	A	450	20.552	94.014	20.503	1.00	52.16
	806	CB	THR	A	450	22.023	93.560	20.501	1.00	53.90
	807	OG1	THR	A	450	22.078	92.132	20.415	1.00	61.82
	808	CG2	THR	A	450	22.723	94.006	21.773	1.00	62.58
	809	C	THR	A	450	20.503	95.547	20.493	1.00	54.69
	810	O	THR	A	450	20.617	96.179	19.441	1.00	51.28
	811	N	PRO	A	451	20.320	96.161	21.669	1.00	57.24
	812	CD	PRO	A	451	19.982	95.539	22.963	1.00	60.66
	813	CA	PRO	A	451	20.261	97.623	21.762	1.00	61.04
	814	CB	PRO	A	451	20.029	97.864	23.254	1.00	61.38
	815	CG	PRO	A	451	19.240	96.654	23.667	1.00	63.63
	816	C	PRO	A	451	21.537	98.299	21.253	1.00	63.11
	817	O	PRO	A	451	22.651	97.918	21.616	1.00	61.66
	818	N	GLU	A	452	21.370	99.297	20.394	1.00	66.04
	819	CA	GLU	A	452	22.517	100.025	19.863	1.00	69.40
	820	CB	GLU	A	452	22.646	99.800	18.347	1.00	67.34
	821	CG	GLU	A	452	24.095	99.689	17.823	1.00	60.86
	822	CD	GLU	A	452	24.785	98.375	18.224	1.00	59.08
	823	OE1	GLU	A	452	24.090	97.345	18.325	1.00	62.62
	824	OE2	GLU	A	452	26.022	98.351	18.424	1.00	45.82
	825	C	GLU	A	452	22.322	101.510	20.170	1.00	71.98
	826	O	GLU	A	452	21.705	102.240	19.395	1.00	70.35
	827	N	ALA	A	453	22.842	101.941	21.317	1.00	75.33
	828	CA	ALA	A	453	22.733	103.334	21.753	1.00	78.80
	829	CB	ALA	A	453	23.482	103.525	23.071	1.00	80.74
	830	C	ALA	A	453	23.260	104.318	20.706	1.00	80.53
	831	O	ALA	A	453	24.167	104.001	19.933	1.00	82.95
	832	N	LYS	A	459	29.802	96.915	16.453	1.00	51.87
	833	CA	LYS	A	459	28.953	96.350	15.407	1.00	52.84
	834	CB	LYS	A	459	29.613	95.121	14.783	1.00	55.20
	835	CG	LYS	A	459	30.879	95.429	14.011	1.00	63.98
	836	CD	LYS	A	459	31.199	94.329	13.012	1.00	72.67
	837	CE	LYS	A	459	30.116	94.234	11.943	1.00	77.63
	838	NZ	LYS	A	459	30.478	93.298	10.841	1.00	83.78
	839	C	LYS	A	459	27.567	95.962	15.905	1.00	50.86
	840	O	LYS	A	459	27.426	95.389	16.982	1.00	49.65
	841	N	ARG	A	460	26.555	96.268	15.099	1.00	48.30
	842	CA	ARG	A	460	25.167	95.960	15.426	1.00	47.61
	843	CB	ARG	A	460	24.250	96.735	14.480	1.00	51.65
	844	CG	ARG	A	460	24.571	98.229	14.509	1.00	59.85
	845	CD	ARG	A	460	23.816	99.030	13.465	1.00	65.41
	846	NE	ARG	A	460	24.200	100.442	13.497	1.00	70.36
	847	CZ	ARG	A	460	25.426	100.898	13.252	1.00	73.06
	848	NH1	ARG	A	460	26.412	100.060	12.950	1.00	75.61
	849	NH2	ARG	A	460	25.671	102.199	13.309	1.00	76.52
	850	C	ARG	A	460	24.936	94.446	15.341	1.00	44.39
	851	O	ARG	A	460	25.542	93.761	14.511	1.00	41.11
	852	N	THR	A	461	24.060	93.928	16.195	1.00	40.18
	853	CA	THR	A	461	23.832	92.489	16.250	1.00	40.02
	854	CB	THR	A	461	24.615	91.867	17.441	1.00	41.84
	855	OG1	THR	A	461	25.999	92.217	17.350	1.00	52.98
	856	CG2	THR	A	461	24.498	90.362	17.434	1.00	48.91
	857	C	THR	A	461	22.393	92.026	16.401	1.00	37.19
	858	O	THR	A	461	21.591	92.641	17.118	1.00	37.94
	859	N	LEU	A	462	22.088	90.919	15.725	1.00	33.00

860	CA	LEU	A	462	20.791	90.265	15.811	1.00	29.46
861	CB	LEU	A	462	20.166	90.050	14.433	1.00	30.35
862	CG	LEU	A	462	19.922	91.318	13.602	1.00	33.09
863	CD1	LEU	A	462	19.188	90.961	12.315	1.00	32.32
864	CD2	LEU	A	462	19.101	92.307	14.401	1.00	25.52
865	C	LEU	A	462	21.161	88.928	16.438	1.00	29.44
866	O	LEU	A	462	22.261	88.416	16.206	1.00	24.62
867	N	ALA	A	463	20.257	88.363	17.232	1.00	27.23
868	CA	ALA	A	463	20.550	87.114	17.908	1.00	27.78
869	CB	ALA	A	463	21.112	87.401	19.310	1.00	26.61
870	C	ALA	A	463	19.299	86.268	17.996	1.00	28.37
871	O	ALA	A	463	18.185	86.776	17.867	1.00	29.09
872	N	CYS	A	464	19.485	84.977	18.230	1.00	22.40
873	CA	CYS	A	464	18.354	84.066	18.279	1.00	26.72
874	C	CYS	A	464	18.562	82.978	19.314	1.00	24.16
875	O	CYS	A	464	19.648	82.401	19.409	1.00	23.01
876	CB	CYS	A	464	18.190	83.428	16.900	1.00	24.58
877	SG	CYS	A	464	16.806	82.273	16.677	1.00	40.31

878	N	LEU	A	465	17.504	82.692	20.068	1.00	22.68
879	CA	LEU	A	465	17.548	81.650	21.087	1.00	24.31
880	CB	LEU	A	465	17.127	82.210	22.460	1.00	26.81
881	CG	LEU	A	465	16.759	81.181	23.546	1.00	21.10
882	CD1	LEU	A	465	17.941	80.290	23.849	1.00	21.73
883	CD2	LEU	A	465	16.338	81.900	24.807	1.00	30.90
884	C	LEU	A	465	16.587	80.557	20.647	1.00	23.79
885	O	LEU	A	465	15.417	80.830	20.359	1.00	22.87
886	N	ILE	A	466	17.079	79.324	20.590	1.00	23.16
887	CA	ILE	A	466	16.251	78.198	20.174	1.00	23.50
888	CB	ILE	A	466	16.762	77.582	18.849	1.00	23.66
889	CG2	ILE	A	466	15.800	76.460	18.395	1.00	29.47
890	CG1	ILE	A	466	16.861	78.687	17.780	1.00	19.89
891	CD1	ILE	A	466	17.371	78.202	16.450	1.00	36.91
892	C	ILE	A	466	16.326	77.212	21.316	1.00	22.24
893	O	ILE	A	466	17.411	76.789	21.715	1.00	24.74
894	N	GLN	A	467	15.167	76.811	21.830	1.00	23.91
895	CA	GLN	A	467	15.182	75.958	23.005	1.00	31.01
896	CB	GLN	A	467	15.224	76.853	24.254	1.00	30.11
897	CG	GLN	A	467	13.993	77.731	24.446	1.00	26.37
898	CD	GLN	A	467	14.114	78.680	25.636	1.00	29.83
899	OE1	GLN	A	467	14.890	78.464	26.579	1.00	28.59
900	NE2	GLN	A	467	13.318	79.731	25.605	1.00	31.49
901	C	GLN	A	467	14.054	74.959	23.148	1.00	33.72
902	O	GLN	A	467	13.131	74.909	22.332	1.00	31.53
903	N	ASN	A	468	14.179	74.158	24.205	1.00	38.27
904	CA	ASN	A	468	13.215	73.135	24.574	1.00	41.08
905	CB	ASN	A	468	11.856	73.761	24.855	1.00	43.70
906	CG	ASN	A	468	11.949	74.935	25.797	1.00	50.48
907	OD1	ASN	A	468	12.641	74.878	26.819	1.00	59.45
908	ND2	ASN	A	468	11.243	76.006	25.472	1.00	56.28
909	C	ASN	A	468	13.052	72.040	23.546	1.00	41.04
910	O	ASN	A	468	11.986	71.445	23.440	1.00	38.53
911	N	PHE	A	469	14.101	71.757	22.791	1.00	38.66
912	CA	PHE	A	469	13.996	70.706	21.797	1.00	38.07
913	CB	PHE	A	469	14.419	71.240	20.427	1.00	29.35
914	CG	PHE	A	469	15.888	71.536	20.309	1.00	28.48
915	CD1	PHE	A	469	16.785	70.541	19.987	1.00	23.56
916	CD2	PHE	A	469	16.369	72.823	20.521	1.00	24.16
917	CE1	PHE	A	469	18.137	70.816	19.872	1.00	27.41
918	CE2	PHE	A	469	17.733	73.107	20.409	1.00	32.69
919	CZ	PHE	A	469	18.616	72.094	20.083	1.00	24.40
920	C	PHE	A	469	14.815	69.475	22.161	1.00	38.11
921	O	PHE	A	469	15.848	69.574	22.813	1.00	39.11

	922	N	MET	A	470	14.333	68.313	21.741	1.00	40.05
	923	CA	MET	A	470	15.001	67.031	21.970	1.00	41.39
	924	CB	MET	A	470	14.618	66.417	23.321	1.00	46.13
	925	CG	MET	A	470	13.159	66.043	23.530	1.00	60.40
	926	SD	MET	A	470	12.863	65.634	25.280	1.00	65.64
	927	CE	MET	A	470	13.541	63.941	25.373	1.00	71.36
	928	C	MET	A	470	14.505	66.183	20.820	1.00	38.04
	929	O	MET	A	470	13.327	66.224	20.482	1.00	36.87
	930	N	PRO	A	471	15.399	65.416	20.175	1.00	37.84
	931	CD	PRO	A	471	14.946	64.687	18.983	1.00	38.40
	932	CA	PRO	A	471	16.853	65.240	20.358	1.00	37.04
	933	CB	PRO	A	471	17.200	64.115	19.368	1.00	38.82
	934	CG	PRO	A	471	15.852	63.524	19.004	1.00	40.26
	935	C	PRO	A	471	17.685	66.508	20.104	1.00	35.06
	936	O	PRO	A	471	17.157	67.524	19.668	1.00	33.27
	937	N	GLU	A	472	18.989	66.420	20.340	1.00	35.63
	938	CA	GLU	A	472	19.895	67.567	20.202	1.00	38.83
	939	CB	GLU	A	472	21.169	67.308	20.991	1.00	43.92
	940	CG	GLU	A	472	22.084	66.301	20.308	1.00	54.98
	941	CD	GLU	A	472	23.312	65.943	21.137	1.00	65.38
	942	OE1	GLU	A	472	23.431	66.428	22.279	1.00	73.96
	943	OE2	GLU	A	472	24.158	65.167	20.650	1.00	71.17
	944	C	GLU	A	472	20.308	68.032	18.806	1.00	36.65
	945	O	GLU	A	472	20.799	69.147	18.649	1.00	32.41
	946	N	ASP	A	473	20.118	67.198	17.789	1.00	35.48
	947	CA	ASP	A	473	20.508	67.596	16.432	1.00	34.00
	948	CB	ASP	A	473	20.534	66.375	15.506	1.00	39.24
	949	CG	ASP	A	473	21.607	65.361	15.907	1.00	48.86
	950	OD1	ASP	A	473	22.724	65.800	16.283	1.00	42.86
	951	OD2	ASP	A	473	21.330	64.139	15.835	1.00	46.87
	952	C	ASP	A	473	19.607	68.683	15.844	1.00	34.33
	953	O	ASP	A	473	18.380	68.543	15.785	1.00	34.18
	954	N	ILE	A	474	20.216	69.776	15.409	1.00	27.93
	955	CA	ILE	A	474	19.435	70.862	14.846	1.00	28.40
	956	CB	ILE	A	474	18.874	71.752	15.971	1.00	25.16
	957	CG2	ILE	A	474	19.998	72.564	16.611	1.00	26.53
	958	CG1	ILE	A	474	17.772	72.665	15.436	1.00	21.56
	959	CD1	ILE	A	474	17.009	73.381	16.593	1.00	23.93
	960	C	ILE	A	474	20.274	71.710	13.910	1.00	26.83
	961	O	ILE	A	474	21.473	71.827	14.086	1.00	25.94
	962	N	SER	A	475	19.625	72.275	12.898	1.00	24.54
	963	CA	SER	A	475	20.264	73.154	11.933	1.00	23.71
	964	CB	SER	A	475	20.014	72.668	10.510	1.00	22.00
	965	OG	SER	A	475	20.555	71.379	10.341	1.00	30.00
	966	C	SER	A	475	19.633	74.529	12.117	1.00	24.55
	967	O	SER	A	475	18.410	74.669	12.135	1.00	23.24
	968	N	VAL	A	476	20.476	75.542	12.253	1.00	24.48
	969	CA	VAL	A	476	20.038	76.908	12.446	1.00	26.25
	970	CB	VAL	A	476	20.672	77.503	13.721	1.00	24.14
	971	CG1	VAL	A	476	20.260	78.965	13.873	1.00	23.36
	972	CG2	VAL	A	476	20.243	76.693	14.937	1.00	28.16
	973	C	VAL	A	476	20.489	77.723	11.253	1.00	28.80
	974	O	VAL	A	476	21.607	77.555	10.761	1.00	32.13
	975	N	GLN	A	477	19.629	78.607	10.774	1.00	28.79
	976	CA	GLN	A	477	20.011	79.424	9.642	1.00	30.02
	977	CB	GLN	A	477	19.746	78.687	8.326	1.00	31.30
	978	CG	GLN	A	477	18.330	78.240	8.107	1.00	46.28
	979	CD	GLN	A	477	18.232	77.101	7.093	1.00	49.95
	980	OE1	GLN	A	477	17.145	76.758	6.635	1.00	51.94
	981	NE2	GLN	A	477	19.373	76.503	6.751	1.00	51.51
	982	C	GLN	A	477	19.287	80.744	9.669	1.00	30.41
	983	O	GLN	A	477	18.185	80.843	10.198	1.00	30.03

	984	N	TRP	A	478	19.941	81.759	9.124	1.00	29.86
	985	CA	TRP	A	478	19.390	83.095	9.058	1.00	29.12
	986	CB	TRP	A	478	20.435	84.101	9.521	1.00	31.11
	987	CG	TRP	A	478	20.664	84.073	10.988	1.00	36.98
	988	CD2	TRP	A	478	19.995	84.874	11.968	1.00	34.77
	989	CE2	TRP	A	478	20.516	84.508	13.230	1.00	37.75
	990	CE3	TRP	A	478	18.998	85.858	11.906	1.00	31.61
	991	CD1	TRP	A	478	21.540	83.280	11.668	1.00	35.86
	992	NE1	TRP	A	478	21.458	83.535	13.014	1.00	35.58
	993	CZ2	TRP	A	478	20.079	85.106	14.432	1.00	26.96
	994	CZ3	TRP	A	478	18.561	86.452	13.095	1.00	35.86
	995	CH2	TRP	A	478	19.103	86.069	14.343	1.00	31.66
	996	C	TRP	A	478	18.952	83.425	7.632	1.00	29.01
	997	O	TRP	A	478	19.594	83.020	6.661	1.00	24.19
	998	N	LEU	A	479	17.858	84.164	7.518	1.00	31.15
	999	CA	LEU	A	479	17.325	84.558	6.220	1.00	36.67
	1000	CB	LEU	A	479	16.063	83.763	5.902	1.00	41.07
	1001	CG	LEU	A	479	16.016	82.272	6.233	1.00	48.71
	1002	CD1	LEU	A	479	14.739	81.711	5.660	1.00	57.57
	1003	CD2	LEU	A	479	17.204	81.546	5.645	1.00	56.00
	1004	C	LEU	A	479	16.976	86.044	6.180	1.00	38.99
	1005	O	LEU	A	479	16.602	86.635	7.191	1.00	37.96
	1006	N	HIS	A	480	17.100	86.637	5.004	1.00	42.00
	1007	CA	HIS	A	480	16.766	88.039	4.816	1.00	48.67
	1008	CB	HIS	A	480	17.952	88.816	4.229	1.00	50.22
	1009	CG	HIS	A	480	17.706	90.291	4.086	1.00	53.99
	1010	CD2	HIS	A	480	18.559	91.344	4.107	1.00	56.80
	1011	ND1	HIS	A	480	16.453	90.821	3.861	1.00	54.56
	1012	CE1	HIS	A	480	16.543	92.135	3.752	1.00	60.76
	1013	NE2	HIS	A	480	17.811	92.478	3.897	1.00	59.92
	1014	C	HIS	A	480	15.628	87.975	3.817	1.00	52.66
	1015	O	HIS	A	480	15.823	88.174	2.618	1.00	51.85
	1016	N	ASN	A	481	14.439	87.655	4.320	1.00	58.88
	1017	CA	ASN	A	481	13.261	87.538	3.472	1.00	63.74
	1018	CB	ASN	A	481	13.012	88.837	2.693	1.00	69.70
	1019	CG	ASN	A	481	12.389	89.926	3.539	1.00	76.04
	1020	OD1	ASN	A	481	12.354	91.087	3.138	1.00	80.67
	1021	ND2	ASN	A	481	11.881	89.558	4.708	1.00	82.88
	1022	C	ASN	A	481	13.466	86.418	2.467	1.00	63.93
	1023	O	ASN	A	481	14.198	86.592	1.496	1.00	67.09
	1024	N	GLU	A	482	12.819	85.278	2.701	1.00	62.43
	1025	CA	GLU	A	482	12.885	84.123	1.801	1.00	60.15
	1026	CB	GLU	A	482	11.977	84.375	0.581	1.00	65.85
	1027	CG	GLU	A	482	11.579	85.846	0.393	1.00	78.14
	1028	CD	GLU	A	482	11.654	86.318	-1.044	1.00	84.88
	1029	OE1	GLU	A	482	12.616	85.938	-1.746	1.00	90.19
	1030	OE2	GLU	A	482	10.759	87.082	-1.466	1.00	87.19
	1031	C	GLU	A	482	14.269	83.651	1.314	1.00	54.93
	1032	O	GLU	A	482	14.406	82.516	0.853	1.00	57.04
	1033	N	VAL	A	483	15.295	84.489	1.414	1.00	49.03
	1034	CA	VAL	A	483	16.613	84.089	0.937	1.00	45.46
	1035	CB	VAL	A	483	17.209	85.150	-0.026	1.00	43.71
	1036	CG1	VAL	A	483	17.320	86.501	0.673	1.00	50.19
	1037	CG2	VAL	A	483	18.567	84.687	-0.533	1.00	43.76
	1038	C	VAL	A	483	17.584	83.842	2.078	1.00	43.31
	1039	O	VAL	A	483	17.741	84.676	2.963	1.00	41.21
	1040	N	GLN	A	484	18.238	82.687	2.039	1.00	42.10
	1041	CA	GLN	A	484	19.189	82.297	3.064	1.00	41.31
	1042	CB	GLN	A	484	19.349	80.778	3.053	1.00	46.93

1043	CG	GLN	A	484	20.420	80.262	3.993	1.00	54.66
1044	CD	GLN	A	484	20.428	78.749	4.101	1.00	61.50
1045	OE1	GLN	A	484	21.402	78.158	4.568	1.00	65.59
1046	NE2	GLN	A	484	19.333	78.114	3.684	1.00	62.36
1047	C	GLN	A	484	20.564	82.958	2.959	1.00	40.69
1048	O	GLN	A	484	21.124	83.097	1.868	1.00	39.56
1049	N	LEU	A	485	21.098	83.358	4.111	1.00	34.74
1050	CA	LEU	A	485	22.408	83.998	4.191	1.00	36.73
1051	CB	LEU	A	485	22.511	84.879	5.445	1.00	36.78
1052	CG	LEU	A	485	21.501	86.011	5.643	1.00	38.16
1053	CD1	LEU	A	485	21.769	86.724	6.966	1.00	39.22
1054	CD2	LEU	A	485	21.607	86.969	4.479	1.00	41.68
1055	C	LEU	A	485	23.485	82.923	4.266	1.00	36.82
1056	O	LEU	A	485	23.212	81.795	4.660	1.00	34.53
1057	N	PRO	A	486	24.725	83.258	3.883	1.00	40.02
1058	CD	PRO	A	486	25.251	84.563	3.448	1.00	39.74
1059	CA	PRO	A	486	25.791	82.249	3.949	1.00	45.08
1060	CB	PRO	A	486	27.018	82.994	3.422	1.00	44.97
1061	CG	PRO	A	486	26.457	84.162	2.661	1.00	41.94
1062	C	PRO	A	486	25.971	81.862	5.413	1.00	49.91
1063	O	PRO	A	486	25.830	82.711	6.291	1.00	49.23
1064	N	ASP	A	487	26.291	80.599	5.677	1.00	54.02
1065	CA	ASP	A	487	26.486	80.131	7.046	1.00	58.50
1066	CB	ASP	A	487	26.851	78.647	7.039	1.00	68.77
1067	CG	ASP	A	487	26.662	77.993	8.392	1.00	79.77
1068	OD1	ASP	A	487	27.164	78.545	9.397	1.00	87.08
1069	OD2	ASP	A	487	26.016	76.921	8.448	1.00	87.04
1070	C	ASP	A	487	27.594	80.928	7.746	1.00	57.99
1071	O	ASP	A	487	27.445	81.352	8.898	1.00	58.25
1072	N	ALA	A	488	28.695	81.135	7.029	1.00	55.74
1073	CA	ALA	A	488	29.852	81.861	7.546	1.00	55.27
1074	CB	ALA	A	488	30.833	82.122	6.418	1.00	55.02
1075	C	ALA	A	488	29.511	83.177	8.239	1.00	54.82
1076	O	ALA	A	488	30.326	83.726	8.983	1.00	55.09
1077	N	ARG	A	489	28.307	83.682	8.004	1.00	52.93
1078	CA	ARG	A	489	27.899	84.944	8.599	1.00	48.90
1079	CB	ARG	A	489	26.799	85.571	7.749	1.00	47.45
1080	CG	ARG	A	489	27.336	86.343	6.563	1.00	49.40
1081	CD	ARG	A	489	27.263	87.828	6.844	1.00	52.76
1082	NE	ARG	A	489	26.103	88.426	6.190	1.00	60.57
1083	CZ	ARG	A	489	25.513	89.559	6.560	1.00	60.40
1084	NH1	ARG	A	489	25.959	90.247	7.604	1.00	61.65
1085	NH2	ARG	A	489	24.480	90.013	5.866	1.00	62.45
1086	C	ARG	A	489	27.456	84.894	10.058	1.00	45.96
1087	O	ARG	A	489	27.501	85.912	10.746	1.00	45.86
1088	N	HIS	A	490	27.032	83.733	10.541	1.00	41.69
1089	CA	HIS	A	490	26.580	83.655	11.928	1.00	38.41
1090	CB	HIS	A	490	25.087	83.286	11.997	1.00	39.34
1091	CG	HIS	A	490	24.775	81.897	11.530	1.00	38.03
1092	CD2	HIS	A	490	24.784	80.715	12.189	1.00	41.49
1093	ND1	HIS	A	490	24.443	81.606	10.224	1.00	44.03
1094	CE1	HIS	A	490	24.263	80.302	10.099	1.00	42.68
1095	NE2	HIS	A	490	24.465	79.740	11.277	1.00	46.75
1096	C	HIS	A	490	27.382	82.679	12.778	1.00	37.56
1097	O	HIS	A	490	28.117	81.852	12.260	1.00	38.74
1098	N	SER	A	491	27.241	82.796	14.094	1.00	36.46
1099	CA	SER	A	491	27.926	81.906	15.021	1.00	35.63
1100	CB	SER	A	491	28.940	82.698	15.845	1.00	34.76
1101	OG	SER	A	491	29.650	81.849	16.726	1.00	51.24
1102	C	SER	A	491	26.888	81.245	15.935	1.00	32.46
1103	O	SER	A	491	26.122	81.928	16.618	1.00	34.26

	1104	N	THR	A	492	26.868	79.919	15.946	1.00	30.35
	1105	CA	THR	A	492	25.922	79.147	16.750	1.00	32.31
	1106	CB	THR	A	492	25.104	78.179	15.837	1.00	33.20
	1107	OG1	THR	A	492	24.459	78.933	14.806	1.00	38.93
	1108	CG2	THR	A	492	24.046	77.415	16.622	1.00	30.28
	1109	C	THR	A	492	26.639	78.328	17.835	1.00	32.83
	1110	O	THR	A	492	27.638	77.670	17.565	1.00	34.30
	1111	N	THR	A	493	26.118	78.360	19.058	1.00	32.82
	1112	CA	THR	A	493	26.719	77.610	20.161	1.00	32.09
	1113	CB	THR	A	493	26.254	78.151	21.530	1.00	27.96
	1114	OG1	THR	A	493	24.825	78.059	21.630	1.00	29.42
	1115	CG2	THR	A	493	26.680	79.600	21.694	1.00	21.13
	1116	C	THR	A	493	26.336	76.131	20.067	1.00	34.06
	1117	O	THR	A	493	25.436	75.770	19.317	1.00	31.49
	1118	N	GLN	A	494	27.030	75.282	20.816	1.00	35.84
	1119	CA	GLN	A	494	26.740	73.848	20.824	1.00	40.51
	1120	CB	GLN	A	494	27.929	73.056	21.382	1.00	46.41
	1121	CG	GLN	A	494	29.169	73.078	20.504	1.00	63.89
	1122	CD	GLN	A	494	28.890	72.592	19.093	1.00	72.04
	1123	OE1	GLN	A	494	28.272	71.547	18.894	1.00	77.06
	1124	NE2	GLN	A	494	29.355	73.350	18.104	1.00	81.58
	1125	C	GLN	A	494	25.512	73.596	21.691	1.00	39.51
	1126	O	GLN	A	494	25.304	74.270	22.698	1.00	38.74
	1127	N	PRO	A	495	24.676	72.623	21.305	1.00	38.63
	1128	CD	PRO	A	495	24.687	71.849	20.051	1.00	37.82
	1129	CA	PRO	A	495	23.480	72.330	22.100	1.00	39.10
	1130	CB	PRO	A	495	22.889	71.124	21.391	1.00	37.94
	1131	CG	PRO	A	495	23.255	71.388	19.954	1.00	43.34
	1132	C	PRO	A	495	23.854	72.031	23.549	1.00	41.43
	1133	O	PRO	A	495	24.838	71.346	23.808	1.00	42.40
	1134	N	ARG	A	496	23.086	72.567	24.487	1.00	41.33
	1135	CA	ARG	A	496	23.343	72.343	25.906	1.00	46.41
	1136	CB	ARG	A	496	23.808	73.635	26.574	1.00	44.11
	1137	CG	ARG	A	496	25.263	73.943	26.332	1.00	51.48
	1138	CD	ARG	A	496	25.633	75.331	26.813	1.00	56.73
	1139	NE	ARG	A	496	27.038	75.393	27.197	1.00	63.41
	1140	CZ	ARG	A	496	27.507	74.984	28.373	1.00	59.61
	1141	NH1	ARG	A	496	26.683	74.489	29.286	1.00	60.71
	1142	NH2	ARG	A	496	28.804	75.066	28.634	1.00	67.27
	1143	C	ARG	A	496	22.090	71.835	26.597	1.00	49.11
	1144	O	ARG	A	496	20.989	72.303	26.318	1.00	48.52
	1145	N	LYS	A	497	22.255	70.870	27.492	1.00	53.35
	1146	CA	LYS	A	497	21.116	70.322	28.208	1.00	60.05
	1147	CB	LYS	A	497	21.527	69.101	29.034	1.00	65.19
	1148	CG	LYS	A	497	21.910	67.887	28.212	1.00	75.27
	1149	CD	LYS	A	497	22.255	66.705	29.103	1.00	80.74
	1150	CE	LYS	A	497	22.534	65.470	28.269	1.00	86.89
	1151	NZ	LYS	A	497	22.854	64.278	29.103	1.00	91.84
	1152	C	LYS	A	497	20.546	71.376	29.131	1.00	62.05
	1153	O	LYS	A	497	21.184	72.391	29.403	1.00	61.50
	1154	N	THR	A	498	19.335	71.135	29.604	1.00	66.47
	1155	CA	THR	A	498	18.690	72.060	30.515	1.00	71.47
	1156	CB	THR	A	498	17.417	72.654	29.893	1.00	73.54
	1157	OG1	THR	A	498	17.118	71.981	28.666	1.00	77.08
	1158	CG2	THR	A	498	17.619	74.120	29.609	1.00	75.50
	1159	C	THR	A	498	18.339	71.319	31.794	1.00	72.65
	1160	O	THR	A	498	18.850	70.223	32.037	1.00	72.18
	1161	N	ALA	A	499	17.477	71.918	32.610	1.00	75.02
	1162	CA	ALA	A	499	17.062	71.303	33.867	1.00	77.01
	1163	CB	ALA	A	499	16.508	72.370	34.814	1.00	76.94
	1164	C	ALA	A	499	16.009	70.224	33.607	1.00	77.96
	1165	O	ALA	A	499	15.034	70.099	34.350	1.00	79.10

	1166	N	GLY	A	500	16.214	69.443	32.552	1.00	78.37
	1167	CA	GLY	A	500	15.273	68.390	32.217	1.00	78.64
	1168	C	GLY	A	500	14.392	68.745	31.032	1.00	77.71
	1169	O	GLY	A	500	13.741	67.878	30.447	1.00	78.53
	1170	N	SER	A	501	14.390	70.021	30.661	1.00	76.72
	1171	CA	SER	A	501	13.567	70.501	29.555	1.00	74.10
	1172	CB	SER	A	501	13.017	71.893	29.899	1.00	79.09
	1173	OG	SER	A	501	14.053	72.787	30.276	1.00	82.51
	1174	C	SER	A	501	14.235	70.545	28.176	1.00	70.47
	1175	O	SER	A	501	14.188	71.575	27.499	1.00	71.67
	1176	N	GLY	A	502	14.849	69.435	27.761	1.00	64.36
	1177	CA	GLY	A	502	15.484	69.369	26.447	1.00	55.25
	1178	C	GLY	A	502	16.799	70.111	26.211	1.00	48.43
	1179	O	GLY	A	502	17.669	70.155	27.081	1.00	47.45
	1180	N	PHE	A	503	16.952	70.678	25.015	1.00	41.96
	1181	CA	PHE	A	503	18.175	71.411	24.665	1.00	34.38
	1182	CB	PHE	A	503	18.975	70.675	23.582	1.00	34.97
	1183	CG	PHE	A	503	19.432	69.304	23.979	1.00	28.11
	1184	CD1	PHE	A	503	18.548	68.232	23.974	1.00	36.44
	1185	CD2	PHE	A	503	20.749	69.082	24.348	1.00	30.75
	1186	CE1	PHE	A	503	18.971	66.960	24.338	1.00	37.43
	1187	CE2	PHE	A	503	21.179	67.812	24.716	1.00	40.11
	1188	CZ	PHE	A	503	20.289	66.750	24.709	1.00	37.06
	1189	C	PHE	A	503	17.922	72.825	24.167	1.00	28.77
	1190	O	PHE	A	503	16.816	73.176	23.756	1.00	28.23
	1191	N	PHE	A	504	18.963	73.637	24.213	1.00	24.91
	1192	CA	PHE	A	504	18.887	75.006	23.743	1.00	25.79
	1193	CB	PHE	A	504	18.644	76.006	24.886	1.00	22.02
	1194	CG	PHE	A	504	19.834	76.257	25.774	1.00	30.92
	1195	CD1	PHE	A	504	20.722	77.300	25.499	1.00	32.77
	1196	CD2	PHE	A	504	20.037	75.487	26.919	1.00	34.76
	1197	CE1	PHE	A	504	21.796	77.570	26.349	1.00	29.72
	1198	CE2	PHE	A	504	21.107	75.748	27.774	1.00	33.59
	1199	CZ	PHE	A	504	21.987	76.799	27.480	1.00	34.51
	1200	C	PHE	A	504	20.175	75.328	23.027	1.00	28.90
	1201	O	PHE	A	504	21.222	74.751	23.317	1.00	26.02
	1202	N	VAL	A	505	20.071	76.252	22.080	1.00	25.50
	1203	CA	VAL	A	505	21.196	76.681	21.296	1.00	25.53
	1204	CB	VAL	A	505	21.193	75.891	19.955	1.00	29.70
	1205	CG1	VAL	A	505	20.184	76.476	19.002	1.00	25.34
	1206	CG2	VAL	A	505	22.563	75.837	19.365	1.00	35.22
	1207	C	VAL	A	505	21.015	78.196	21.092	1.00	26.24
	1208	O	VAL	A	505	19.895	78.707	21.096	1.00	22.25
	1209	N	PHE	A	506	22.125	78.913	20.950	1.00	28.62
	1210	CA	PHE	A	506	22.093	80.361	20.754	1.00	25.84
	1211	CB	PHE	A	506	22.769	81.061	21.935	1.00	29.19
	1212	CG	PHE	A	506	22.789	82.547	21.827	1.00	35.82
	1213	CD1	PHE	A	506	21.630	83.286	22.030	1.00	42.42
	1214	CD2	PHE	A	506	23.961	83.213	21.500	1.00	42.16
	1215	CE1	PHE	A	506	21.644	84.671	21.910	1.00	44.85
	1216	CE2	PHE	A	506	23.982	84.591	21.376	1.00	41.56
	1217	CZ	PHE	A	506	22.825	85.322	21.580	1.00	45.90
	1218	C	PHE	A	506	22.844	80.719	19.473	1.00	23.92
	1219	O	PHE	A	506	23.924	80.195	19.225	1.00	27.54
	1220	N	SER	A	507	22.286	81.618	18.677	1.00	25.96
	1221	CA	SER	A	507	22.925	82.041	17.432	1.00	25.75
	1222	CB	SER	A	507	22.144	81.481	16.235	1.00	24.23
	1223	OG	SER	A	507	22.674	81.957	15.012	1.00	33.35
	1224	C	SER	A	507	23.027	83.574	17.364	1.00	25.49
	1225	O	SER	A	507	22.070	84.284	17.648	1.00	25.61
	1226	N	ARG	A	508	24.203	84.063	16.994	1.00	26.99
	1227	CA	ARG	A	508	24.475	85.497	16.907	1.00	25.78

	1228	CB	ARG	A	508	25.652	85.821	17.825	1.00	24.46
	1229	CG	ARG	A	508	26.177	87.245	17.753	1.00	28.19
	1230	CD	ARG	A	508	27.409	87.349	18.638	1.00	27.68
	1231	NE	ARG	A	508	27.865	88.723	18.804	1.00	38.82
	1232	CZ	ARG	A	508	28.641	89.355	17.933	1.00	40.66
	1233	NH1	ARG	A	508	29.046	88.726	16.840	1.00	39.61
	1234	NH2	ARG	A	508	29.007	90.613	18.151	1.00	40.23
	1235	C	ARG	A	508	24.816	85.910	15.471	1.00	24.52
	1236	O	ARG	A	508	25.594	85.234	14.810	1.00	24.88
	1237	N	LEU	A	509	24.246	87.013	14.992	1.00	26.27
	1238	CA	LEU	A	509	24.512	87.490	13.622	1.00	31.33
	1239	CB	LEU	A	509	23.303	87.206	12.721	1.00	32.56
	1240	CG	LEU	A	509	23.311	87.774	11.292	1.00	33.39
	1241	CD1	LEU	A	509	24.350	87.049	10.434	1.00	27.13
	1242	CD2	LEU	A	509	21.921	87.614	10.691	1.00	27.35
	1243	C	LEU	A	509	24.830	88.988	13.550	1.00	33.20
	1244	O	LEU	A	509	23.946	89.823	13.721	1.00	35.36
	1245	N	GLU	A	510	26.091	89.330	13.286	1.00	33.43
	1246	CA	GLU	A	510	26.479	90.735	13.182	1.00	37.45
	1247	CB	GLU	A	510	28.002	90.880	13.305	1.00	38.70
	1248	CG	GLU	A	510	28.548	90.352	14.629	1.00	53.61
	1249	CD	GLU	A	510	30.009	90.722	14.897	1.00	62.03
	1250	OE1	GLU	A	510	30.877	90.439	14.042	1.00	65.31
	1251	OE2	GLU	A	510	30.288	91.290	15.976	1.00	63.62
	1252	C	GLU	A	510	26.007	91.285	11.841	1.00	37.95
	1253	O	GLU	A	510	26.187	90.635	10.808	1.00	35.84
	1254	N	VAL	A	511	25.391	92.466	11.845	1.00	37.36
	1255	CA	VAL	A	511	24.903	93.048	10.596	1.00	39.69
	1256	CB	VAL	A	511	23.366	93.012	10.513	1.00	29.12
	1257	CG1	VAL	A	511	22.875	91.590	10.689	1.00	28.52
	1258	CG2	VAL	A	511	22.764	93.933	11.554	1.00	31.67
	1259	C	VAL	A	511	25.357	94.490	10.392	1.00	45.51
	1260	O	VAL	A	511	25.776	95.156	11.344	1.00	46.84
	1261	N	THR	A	512	25.269	94.964	9.150	1.00	47.32
	1262	CA	THR	A	512	25.673	96.326	8.813	1.00	51.20
	1263	CB	THR	A	512	25.922	96.471	7.304	1.00	49.91
	1264	OG1	THR	A	512	24.723	96.142	6.592	1.00	46.57
	1265	CG2	THR	A	512	27.046	95.544	6.858	1.00	49.02
	1266	C	THR	A	512	24.585	97.312	9.213	1.00	54.77
	1267	O	THR	A	512	23.467	96.909	9.520	1.00	54.38
	1268	N	ARG	A	513	24.916	98.602	9.206	1.00	56.48
	1269	CA	ARG	A	513	23.955	99.642	9.565	1.00	56.58
	1270	CB	ARG	A	513	24.609	101.026	9.503	1.00	61.58
	1271	CG	ARG	A	513	24.030	102.030	10.489	1.00	67.62
	1272	CD	ARG	A	513	22.566	102.306	10.221	1.00	75.58
	1273	NE	ARG	A	513	21.857	102.737	11.422	1.00	83.06
	1274	CZ	ARG	A	513	20.572	103.081	11.448	1.00	86.37
	1275	NH1	ARG	A	513	19.856	103.049	10.336	1.00	88.41
	1276	NH2	ARG	A	513	19.998	103.446	12.585	1.00	87.87
	1277	C	ARG	A	513	22.783	99.603	8.600	1.00	55.15
	1278	O	ARG	A	513	21.639	99.856	8.983	1.00	55.55
	1279	N	ALA	A	514	23.076	99.281	7.345	1.00	55.02
	1280	CA	ALA	A	514	22.055	99.214	6.308	1.00	53.96
	1281	CB	ALA	A	514	22.715	98.972	4.961	1.00	53.56
	1282	C	ALA	A	514	21.015	98.128	6.595	1.00	54.12
	1283	O	ALA	A	514	19.819	98.413	6.681	1.00	54.41
	1284	N	GLU	A	515	21.464	96.884	6.736	1.00	54.63
	1285	CA	GLU	A	515	20.535	95.798	7.011	1.00	54.64
	1286	CB	GLU	A	515	21.225	94.434	6.862	1.00	58.15
	1287	CG	GLU	A	515	22.668	94.392	7.331	1.00	64.48
	1288	CD	GLU	A	515	23.379	93.107	6.926	1.00	65.38
	1289	OE1	GLU	A	515	23.183	92.643	5.784	1.00	66.84

	1290	OE2	GLU	A	515	24.149	92.563	7.741	1.00	68.35
	1291	C	GLU	A	515	19.929	95.956	8.395	1.00	54.36
	1292	O	GLU	A	515	18.897	95.360	8.694	1.00	51.06
	1293	N	TRP	A	516	20.563	96.769	9.237	1.00	55.85
	1294	CA	TRP	A	516	20.043	97.015	10.576	1.00	57.10
	1295	CB	TRP	A	516	21.062	97.755	11.447	1.00	58.50
	1296	CG	TRP	A	516	20.726	97.650	12.906	1.00	67.12
	1297	CD2	TRP	A	516	20.128	98.660	13.726	1.00	68.04
	1298	CE2	TRP	A	516	19.915	98.091	14.999	1.00	71.07
	1299	CE3	TRP	A	516	19.751	99.992	13.507	1.00	74.06
	1300	CD1	TRP	A	516	20.851	96.541	13.697	1.00	67.58
	1301	NE1	TRP	A	516	20.364	96.797	14.954	1.00	68.75
	1302	CZ2	TRP	A	516	19.337	98.807	16.052	1.00	75.59
	1303	CZ3	TRP	A	516	19.175	100.705	14.558	1.00	76.50
	1304	CH2	TRP	A	516	18.975	100.109	15.813	1.00	76.13
	1305	C	TRP	A	516	18.772	97.854	10.452	1.00	57.68
	1306	O	TRP	A	516	17.909	97.825	11.327	1.00	57.71
	1307	N	GLU	A	517	18.665	98.604	9.357	1.00	58.53
	1308	CA	GLU	A	517	17.487	99.427	9.092	1.00	60.83
	1309	CB	GLU	A	517	17.758	100.381	7.921	1.00	65.68
	1310	CG	GLU	A	517	18.237	101.768	8.325	1.00	77.69
	1311	CD	GLU	A	517	17.213	102.522	9.168	1.00	86.61
	1312	OE1	GLU	A	517	16.066	102.036	9.301	1.00	92.24
	1313	OE2	GLU	A	517	17.550	103.605	9.696	1.00	89.43
	1314	C	GLU	A	517	16.277	98.547	8.755	1.00	58.89
	1315	O	GLU	A	517	15.135	98.871	9.088	1.00	56.98
	1316	N	ALA	A	518	16.537	97.430	8.084	1.00	58.33
	1317	CA	ALA	A	518	15.479	96.503	7.702	1.00	54.78
	1318	CB	ALA	A	518	15.595	96.178	6.220	1.00	55.11
	1319	C	ALA	A	518	15.597	95.227	8.540	1.00	53.56
	1320	O	ALA	A	518	15.375	94.120	8.045	1.00	52.54
	1321	N	LYS	A	519	15.919	95.381	9.819	1.00	51.73
	1322	CA	LYS	A	519	16.092	94.217	10.671	1.00	52.62
	1323	CB	LYS	A	519	16.719	94.617	12.004	1.00	52.68
	1324	CG	LYS	A	519	15.808	95.347	12.954	1.00	53.71
	1325	CD	LYS	A	519	16.631	95.904	14.103	1.00	61.43
	1326	CE	LYS	A	519	15.781	96.701	15.064	1.00	65.64
	1327	NZ	LYS	A	519	16.642	97.460	16.002	1.00	74.93
	1328	C	LYS	A	519	14.814	93.440	10.915	1.00	52.55
	1329	O	LYS	A	519	14.857	92.287	11.339	1.00	49.84
	1330	N	ASP	A	520	13.680	94.067	10.638	1.00	54.27
	1331	CA	ASP	A	520	12.381	93.424	10.820	1.00	55.54
	1332	CB	ASP	A	520	11.263	94.454	10.669	1.00	65.40
	1333	CG	ASP	A	520	11.743	95.878	10.904	1.00	75.80
	1334	OD1	ASP	A	520	12.217	96.174	12.024	1.00	83.22
	1335	OD2	ASP	A	520	11.652	96.700	9.964	1.00	77.87
	1336	C	ASP	A	520	12.212	92.345	9.754	1.00	53.46
	1337	O	ASP	A	520	11.319	91.500	9.843	1.00	51.37
	1338	N	GLU	A	521	13.079	92.383	8.747	1.00	50.72
	1339	CA	GLU	A	521	13.016	91.422	7.658	1.00	50.66
	1340	CB	GLU	A	521	13.427	92.093	6.342	1.00	54.68
	1341	CG	GLU	A	521	12.408	93.090	5.799	1.00	61.75
	1342	CD	GLU	A	521	12.961	93.937	4.670	1.00	68.36
	1343	OE1	GLU	A	521	13.463	93.368	3.678	1.00	70.14
	1344	OE2	GLU	A	521	12.892	95.181	4.773	1.00	75.93
	1345	C	GLU	A	521	13.869	90.182	7.885	1.00	46.52
	1346	O	GLU	A	521	13.743	89.208	7.148	1.00	47.21
	1347	N	PHE	A	522	14.734	90.214	8.893	1.00	42.97
	1348	CA	PHE	A	522	15.589	89.069	9.181	1.00	38.46
	1349	CB	PHE	A	522	16.848	89.509	9.915	1.00	37.28
	1350	CG	PHE	A	522	17.846	90.180	9.024	1.00	42.52
	1351	CD1	PHE	A	522	17.675	91.510	8.646	1.00	44.12

	1352	CD2	PHE	A	522	18.929	89.467	8.508	1.00	40.14
	1353	CE1	PHE	A	522	18.564	92.126	7.762	1.00	48.02
	1354	CE2	PHE	A	522	19.825	90.072	7.623	1.00	42.77
	1355	CZ	PHE	A	522	19.640	91.408	7.248	1.00	41.32
	1356	C	PHE	A	522	14.852	88.006	9.970	1.00	36.02
	1357	O	PHE	A	522	14.126	88.308	10.918	1.00	37.87
	1358	N	ILE	A	523	15.042	86.758	9.561	1.00	32.13
	1359	CA	ILE	A	523	14.376	85.626	10.187	1.00	31.74
	1360	CB	ILE	A	523	13.392	84.966	9.192	1.00	36.58
	1361	CG2	ILE	A	523	12.711	83.751	9.838	1.00	38.36
	1362	CG1	ILE	A	523	12.367	86.000	8.714	1.00	39.38
	1363	CD1	ILE	A	523	11.517	85.514	7.564	1.00	40.35
	1364	C	ILE	A	523	15.356	84.559	10.670	1.00	30.51
	1365	O	ILE	A	523	16.369	84.294	10.034	1.00	29.34
	1366	N	CYS	A	524	15.046	83.949	11.802	1.00	28.73
	1367	CA	CYS	A	524	15.879	82.898	12.351	1.00	27.60
	1368	C	CYS	A	524	15.081	81.635	12.136	1.00	27.54
	1369	O	CYS	A	524	13.933	81.567	12.555	1.00	28.72
	1370	CB	CYS	A	524	16.096	83.123	13.849	1.00	26.75
	1371	SG	CYS	A	524	16.999	81.777	14.689	1.00	36.31
	1372	N	ARG	A	525	15.675	80.636	11.497	1.00	28.42
	1373	CA	ARG	A	525	14.966	79.400	11.226	1.00	28.35
	1374	CB	ARG	A	525	14.780	79.229	9.720	1.00	34.16
	1375	CG	ARG	A	525	14.120	77.912	9.331	1.00	39.75
	1376	CD	ARG	A	525	13.508	77.996	7.937	1.00	48.43
	1377	NE	ARG	A	525	14.483	77.825	6.874	1.00	52.97
	1378	CZ	ARG	A	525	14.242	78.108	5.598	1.00	58.72
	1379	NH1	ARG	A	525	13.054	78.580	5.233	1.00	55.56
	1380	NH2	ARG	A	525	15.190	77.930	4.686	1.00	55.90
	1381	C	ARG	A	525	15.673	78.184	11.783	1.00	28.14
	1382	O	ARG	A	525	16.889	78.055	11.691	1.00	28.95
	1383	N	ALA	A	526	14.892	77.283	12.357	1.00	25.82
	1384	CA	ALA	A	526	15.440	76.082	12.930	1.00	25.90
	1385	CB	ALA	A	526	15.056	75.986	14.409	1.00	28.82
	1386	C	ALA	A	526	14.871	74.903	12.169	1.00	27.38
	1387	O	ALA	A	526	13.690	74.899	11.847	1.00	24.32
	1388	N	VAL	A	527	15.718	73.924	11.855	1.00	24.37
	1389	CA	VAL	A	527	15.266	72.727	11.177	1.00	24.12
	1390	CB	VAL	A	527	16.054	72.434	9.899	1.00	24.30
	1391	CG1	VAL	A	527	15.637	71.090	9.338	1.00	26.10
	1392	CG2	VAL	A	527	15.796	73.517	8.876	1.00	30.97
	1393	C	VAL	A	527	15.523	71.646	12.198	1.00	26.78
	1394	O	VAL	A	527	16.631	71.522	12.725	1.00	25.10
	1395	N	HIS	A	528	14.497	70.857	12.470	1.00	26.18
	1396	CA	HIS	A	528	14.585	69.829	13.484	1.00	29.17
	1397	CB	HIS	A	528	14.413	70.490	14.879	1.00	28.69
	1398	CG	HIS	A	528	14.409	69.522	16.028	1.00	30.83
	1399	CD2	HIS	A	528	13.456	68.661	16.461	1.00	30.29
	1400	ND1	HIS	A	528	15.504	69.318	16.842	1.00	30.55
	1401	CE1	HIS	A	528	15.228	68.367	17.719	1.00	28.76
	1402	NE2	HIS	A	528	13.992	67.950	17.507	1.00	23.82
	1403	C	HIS	A	528	13.498	68.782	13.230	1.00	31.62
	1404	O	HIS	A	528	12.387	69.096	12.788	1.00	30.62
	1405	N	GLU	A	529	13.834	67.539	13.543	1.00	34.89
	1406	CA	GLU	A	529	12.949	66.400	13.347	1.00	41.27
	1407	CB	GLU	A	529	13.640	65.129	13.843	1.00	46.90
	1408	CG	GLU	A	529	12.721	63.908	13.872	1.00	61.52
	1409	CD	GLU	A	529	13.184	62.836	14.852	1.00	68.52
	1410	OE1	GLU	A	529	12.433	61.860	15.064	1.00	68.05
	1411	OE2	GLU	A	529	14.294	62.969	15.413	1.00	73.22
	1412	C	GLU	A	529	11.565	66.476	13.996	1.00	42.79
	1413	O	GLU	A	529	10.578	66.069	13.381	1.00	42.08

	1414	N	ALA	A	530	11.502	66.978	15.232	1.00	43.28
	1415	CA	ALA	A	530	10.250	67.061	15.987	1.00	44.89
	1416	CB	ALA	A	530	10.546	67.183	17.472	1.00	42.67
	1417	C	ALA	A	530	9.263	68.142	15.582	1.00	47.12
	1418	O	ALA	A	530	8.126	68.137	16.048	1.00	47.05
	1419	N	ALA	A	531	9.684	69.071	14.732	1.00	50.02
	1420	CA	ALA	A	531	8.792	70.130	14.280	1.00	54.71
	1421	CB	ALA	A	531	9.602	71.233	13.621	1.00	52.38
	1422	C	ALA	A	531	7.787	69.519	13.292	1.00	59.71
	1423	O	ALA	A	531	7.784	69.835	12.102	1.00	57.91
	1424	N	SER	A	532	6.936	68.642	13.825	1.00	66.39
	1425	CA	SER	A	532	5.911	67.899	13.078	1.00	71.61
	1426	CB	SER	A	532	4.570	67.949	13.828	1.00	75.15
	1427	OG	SER	A	532	4.190	69.274	14.168	1.00	81.74
	1428	C	SER	A	532	5.681	68.198	11.595	1.00	73.08
	1429	O	SER	A	532	5.855	67.307	10.757	1.00	75.98
	1430	N	PRO	A	533	5.279	69.433	11.236	1.00	72.21
	1431	CD	PRO	A	533	4.769	70.589	11.998	1.00	72.93
	1432	CA	PRO	A	533	5.076	69.644	9.801	1.00	69.88
	1433	CB	PRO	A	533	3.913	70.617	9.775	1.00	69.60
	1434	CG	PRO	A	533	4.278	71.537	10.895	1.00	71.96
	1435	C	PRO	A	533	6.317	70.212	9.113	1.00	67.12
	1436	O	PRO	A	533	6.820	71.269	9.500	1.00	67.77
	1437	N	SER	A	534	6.802	69.499	8.103	1.00	62.96
	1438	CA	SER	A	534	7.967	69.917	7.331	1.00	56.20
	1439	CB	SER	A	534	7.609	71.137	6.479	1.00	57.74
	1440	OG	SER	A	534	6.985	72.137	7.262	1.00	67.85
	1441	C	SER	A	534	9.258	70.194	8.111	1.00	49.03
	1442	O	SER	A	534	10.176	70.811	7.576	1.00	47.21
	1443	N	GLN	A	535	9.322	69.742	9.363	1.00	42.33
	1444	CA	GLN	A	535	10.504	69.896	10.204	1.00	38.93
	1445	CB	GLN	A	535	11.588	68.887	9.784	1.00	32.30
	1446	CG	GLN	A	535	11.212	67.419	9.972	1.00	35.25
	1447	CD	GLN	A	535	10.074	66.981	9.076	1.00	41.01
	1448	OE1	GLN	A	535	10.112	67.172	7.861	1.00	43.29
	1449	NE2	GLN	A	535	9.055	66.380	9.669	1.00	47.79
	1450	C	GLN	A	535	11.115	71.290	10.209	1.00	37.85
	1451	O	GLN	A	535	12.335	71.432	10.281	1.00	36.76
	1452	N	THR	A	536	10.280	72.317	10.147	1.00	37.28
	1453	CA	THR	A	536	10.795	73.675	10.145	1.00	39.00
	1454	CB	THR	A	536	10.752	74.281	8.734	1.00	41.53
	1455	OG1	THR	A	536	11.256	73.333	7.786	1.00	46.75
	1456	CG2	THR	A	536	11.613	75.524	8.676	1.00	39.44
	1457	C	THR	A	536	10.014	74.584	11.072	1.00	38.42
	1458	O	THR	A	536	8.806	74.452	11.205	1.00	43.26
	1459	N	VAL	A	537	10.723	75.495	11.726	1.00	37.42
	1460	CA	VAL	A	537	10.138	76.469	12.632	1.00	32.52
	1461	CB	VAL	A	537	10.134	75.981	14.110	1.00	36.29
	1462	CG1	VAL	A	537	9.452	77.020	14.986	1.00	35.71
	1463	CG2	VAL	A	537	9.395	74.669	14.241	1.00	43.42
	1464	C	VAL	A	537	11.006	77.724	12.538	1.00	31.41
	1465	O	VAL	A	537	12.231	77.654	12.665	1.00	31.67
	1466	N	GLN	A	538	10.381	78.874	12.313	1.00	27.91
	1467	CA	GLN	A	538	11.148	80.104	12.183	1.00	29.41
	1468	CB	GLN	A	538	11.464	80.369	10.708	1.00	29.17
	1469	CG	GLN	A	538	10.237	80.635	9.849	1.00	29.81
	1470	CD	GLN	A	538	10.617	80.890	8.409	1.00	29.58
	1471	OE1	GLN	A	538	11.424	80.157	7.833	1.00	37.40
	1472	NE2	GLN	A	538	10.041	81.924	7.815	1.00	32.13
	1473	C	GLN	A	538	10.407	81.296	12.744	1.00	31.40
	1474	O	GLN	A	538	9.189	81.286	12.844	1.00	33.62
	1475	N	ARG	A	539	11.151	82.333	13.098	1.00	31.64

	1476	CA	ARG	A	539	10.537	83.534	13.619	1.00	34.86
	1477	CB	ARG	A	539	10.480	83.480	15.145	1.00	41.64
	1478	CG	ARG	A	539	9.522	84.477	15.762	1.00	48.95
	1479	CD	ARG	A	539	8.755	83.804	16.884	1.00	59.63
	1480	NE	ARG	A	539	8.205	82.533	16.420	1.00	74.02
	1481	CZ	ARG	A	539	7.506	81.691	17.173	1.00	82.05
	1482	NH1	ARG	A	539	7.259	81.977	18.447	1.00	87.03
	1483	NH2	ARG	A	539	7.053	80.560	16.646	1.00	85.40
	1484	C	ARG	A	539	11.311	84.760	13.178	1.00	34.74
	1485	O	ARG	A	539	12.541	84.767	13.190	1.00	37.29
	1486	N	ALA	A	540	10.580	85.794	12.772	1.00	34.85
	1487	CA	ALA	A	540	11.192	87.039	12.344	1.00	34.24
	1488	CB	ALA	A	540	10.175	87.891	11.628	1.00	35.02
	1489	C	ALA	A	540	11.700	87.754	13.587	1.00	35.51
	1490	O	ALA	A	540	11.205	87.518	14.695	1.00	30.77
	1491	N	VAL	A	541	12.704	88.604	13.408	1.00	36.19
	1492	CA	VAL	A	541	13.274	89.349	14.520	1.00	42.85
	1493	CB	VAL	A	541	14.428	90.265	14.038	1.00	43.71
	1494	CG1	VAL	A	541	14.744	91.316	15.084	1.00	48.75
	1495	CG2	VAL	A	541	15.665	89.433	13.749	1.00	43.59
	1496	C	VAL	A	541	12.181	90.194	15.178	1.00	48.00
	1497	O	VAL	A	541	11.587	91.063	14.536	1.00	44.96
	1498	N	SER	A	542	11.906	89.927	16.451	1.00	53.41
	1499	CA	SER	A	542	10.883	90.686	17.152	1.00	61.94
	1500	CB	SER	A	542	10.532	90.036	18.494	1.00	62.96
	1501	OG	SER	A	542	11.596	90.138	19.421	1.00	69.91
	1502	C	SER	A	542	11.437	92.083	17.372	1.00	65.98
	1503	O	SER	A	542	12.628	92.253	17.634	1.00	67.12
	1504	N	VAL	A	543	10.571	93.080	17.249	1.00	70.21
	1505	CA	VAL	A	543	10.975	94.466	17.421	1.00	74.63
	1506	CB	VAL	A	543	11.300	95.121	16.058	1.00	78.23
	1507	CG1	VAL	A	543	11.713	96.574	16.260	1.00	79.65
	1508	CG2	VAL	A	543	12.409	94.344	15.359	1.00	79.80
	1509	C	VAL	A	543	9.871	95.259	18.111	1.00	75.67
	1510	O	VAL	A	543	8.974	95.753	17.396	1.00	77.58
	1511	OXT	VAL	A	543	9.907	95.360	19.356	1.00	74.95
	1512	C1	NAG	A	2	39.866	71.246	15.298	1.00	97.60
	1513	O1	NAG	A	2	39.913	72.355	16.125	1.00	99.81
	1514	C2	NAG	A	2	38.452	71.095	14.687	1.00	96.75
	1515	N2	NAG	A	2	38.075	72.305	13.989	1.00	98.55
	1516	C7	NAG	A	2	38.040	72.336	12.660	1.00	101.24
	1517	O7	NAG	A	2	38.381	71.385	11.956	1.00	100.19
	1518	C8	NAG	A	2	37.567	73.623	12.006	1.00	100.76
	1519	C3	NAG	A	2	37.394	70.819	15.772	1.00	96.21
	1520	O3	NAG	A	2	36.138	70.525	15.162	1.00	95.30
	1521	C4	NAG	A	2	37.840	69.634	16.642	1.00	94.75
	1522	O4	NAG	A	2	36.924	69.444	17.725	1.00	91.92
	1523	C5	NAG	A	2	39.273	69.896	17.179	1.00	95.52
	1524	O5	NAG	A	2	40.204	70.093	16.083	1.00	96.34
	1525	C6	NAG	A	2	39.775	68.727	17.999	1.00	96.13
	1526	O6	NAG	A	2	39.723	67.507	17.266	1.00	99.34
	1527	OH2	TIP	A	1	24.621	77.330	12.183	1.00	50.26
	1528	OH2	TIP	A	2	17.289	54.802	2.062	1.00	49.71
	1529	OH2	TIP	A	3	10.654	89.058	-3.198	1.00	62.73
	1530	OH2	TIP	A	4	22.344	80.875	7.156	1.00	44.66
	1531	OH2	TIP	A	5	27.537	65.331	9.249	1.00	53.56
	1532	OH2	TIP	A	6	26.192	96.403	20.749	1.00	44.98
	1533	OH2	TIP	A	7	8.855	79.202	17.894	1.00	44.08
	1534	OH2	TIP	A	8	16.591	66.982	14.521	1.00	40.39
	1535	OH2	TIP	A	9	24.434	65.928	6.674	1.00	40.49
	1536	OH2	TIP	A	10	27.385	88.484	9.939	1.00	46.89
	1537	OH2	TIP	A	11	28.304	87.357	13.183	1.00	50.51

	1538	OH2	TIP	A	12	28.907	78.522	14.088	1.00	50.17
	1539	OH2	TIP	A	13	47.570	70.510	13.386	1.00	54.70
	1540	OH2	TIP	A	14	23.814	76.382	23.745	1.00	44.57
	1541	OH2	TIP	A	15	22.971	61.676	0.664	1.00	50.94
	1542	OH2	TIP	A	16	19.616	104.062	18.276	1.00	56.21
	1543	OH2	TIP	A	17	30.294	75.010	30.820	1.00	59.52
	1544	OH2	TIP	A	18	10.090	82.420	4.828	1.00	55.58
	1545	OH2	TIP	A	19	45.243	73.089	9.124	1.00	66.56
	1546	OH2	TIP	A	20	46.743	70.603	11.012	1.00	63.77
	1547	OH2	TIP	A	21	29.058	92.561	8.613	1.00	62.34
	1548	OH2	TIP	A	22	26.556	59.226	16.825	1.00	54.44
	1549	OH2	TIP	A	23	26.041	54.669	2.219	1.00	52.42
	1550	OH2	TIP	A	24	34.966	68.214	16.774	1.00	60.14
	1551	OH2	TIP	A	25	20.048	55.636	12.052	1.00	48.11
	1552	OH2	TIP	A	26	28.830	86.081	15.665	1.00	45.10
	1553	OH2	TIP	A	27	34.158	69.085	18.975	1.00	59.32
	1554	OH2	TIP	A	28	28.875	47.094	5.425	1.00	53.61
	1555	OH2	TIP	A	29	26.558	67.506	3.036	1.00	60.13
	1556	OH2	TIP	A	30	38.399	52.730	18.974	1.00	56.34
	1557	OH2	TIP	A	31	23.500	72.144	10.139	1.00	58.14
	1558	OH2	TIP	A	32	34.771	64.807	3.542	1.00	50.57
	1559	OH2	TIP	A	33	24.268	95.724	3.944	1.00	56.48
	1560	OH2	TIP	A	34	27.690	78.824	11.826	1.00	60.64
	1561	OH2	TIP	A	35	49.321	73.518	9.173	1.00	56.75
	1562	OH2	TIP	A	36	20.391	63.685	13.114	1.00	52.49
	1563	OH2	TIP	A	37	25.216	70.518	28.590	1.00	56.17
	1564	OH2	TIP	A	38	42.408	48.356	24.205	1.00	57.49
	1565	OH2	TIP	A	39	29.180	99.267	16.299	1.00	59.27
	1566	OH2	TIP	A	40	14.998	75.915	2.509	1.00	55.17
	1567	OH2	TIP	A	41	25.941	69.212	22.056	1.00	55.25
	1568	OH2	TIP	A	42	11.307	86.566	17.528	1.00	50.93
	1569	OH2	TIP	A	43	26.577	64.924	15.413	1.00	58.05
	1570	OH2	TIP	A	44	9.305	75.672	24.091	1.00	63.22
	1571	OH2	TIP	A	45	31.263	91.102	9.512	1.00	59.76
	1572	OH2	TIP	A	46	29.116	71.553	15.523	1.00	61.09
	1573	OH2	TIP	A	47	20.286	50.431	1.295	1.00	58.75
	1574	OH2	TIP	A	48	39.170	57.553	3.300	1.00	59.73
	1575	OH2	TIP	A	49	8.842	71.660	23.296	1.00	53.77
	1576	OH2	TIP	A	50	12.559	48.527	9.562	1.00	59.31
	1577	OH2	TIP	A	51	28.206	76.115	14.977	1.00	56.85
	1578	OH2	TIP	A	52	8.825	77.060	27.183	1.00	60.05
	1579	OH2	TIP	A	53	32.649	60.706	17.690	1.00	57.10
	1580	OH2	TIP	A	54	49.662	60.238	13.997	1.00	60.54
	1581	OH2	TIP	A	55	30.363	57.461	17.811	1.00	62.47
	1582	OH2	TIP	A	56	24.541	106.634	19.860	1.00	64.33
	1583	OH2	TIP	A	57	11.412	70.168	26.131	1.00	52.42
	1584	OH2	TIP	A	58	10.025	88.314	3.596	1.00	60.20
	1585	OH2	TIP	A	59	22.043	63.628	26.199	1.00	59.26
	1586	OH2	TIP	A	60	46.414	76.131	6.439	1.00	62.09
	1587	OH2	TIP	A	61	22.767	54.070	3.523	1.00	65.16
	1588	OH2	TIP	A	62	14.610	78.959	1.837	1.00	59.85
	1589	OH2	TIP	A	63	18.102	59.201	0.758	1.00	56.88
	1590	OH2	TIP	A	64	29.616	80.265	4.265	1.00	53.06
	1591	OH2	TIP	A	65	18.383	97.407	19.064	1.00	60.26
	1592	OH2	TIP	A	66	16.855	77.568	2.254	1.00	59.03
	1593	OH2	TIP	A	67	32.757	64.887	12.306	1.00	54.95
	1594	OH2	TIP	A	68	27.226	97.417	12.532	1.00	57.65
	1595	OH2	TIP	A	69	16.812	67.479	30.053	1.00	59.41

	1596	OH2	TIP	A	70	12.053	64.929	3.775	1.00	62.27
	1597	OH2	TIP	A	71	36.626	74.187	14.978	1.00	55.86
	1598	OH2	TIP	A	72	33.116	54.343	0.777	1.00	59.39
	1599	OH2	TIP	A	73	21.701	75.116	6.786	1.00	59.25
	1600	OH2	TIP	A	74	33.920	50.039	9.248	1.00	53.17
	1601	OH2	TIP	A	75	10.687	52.377	4.811	1.00	65.55
	1602	OH2	TIP	A	76	41.791	50.133	21.910	1.00	62.05
	1603	OH2	TIP	A	77	38.603	74.281	16.682	1.00	57.87
	1604	OH2	TIP	A	78	11.460	76.303	28.686	1.00	58.31
	1605	OH2	TIP	A	79	22.506	95.718	17.568	1.00	53.97
	1606	OH2	TIP	A	80	20.912	49.812	13.914	1.00	54.45
	1607	OH2	TIP	A	81	21.594	91.198	3.704	1.00	60.50
	1608	OH2	TIP	A	82	5.956	84.199	15.573	1.00	54.25
	1609	OH2	TIP	A	83	6.295	66.853	17.967	1.00	58.03
	1610	OH2	TIP	A	84	13.965	68.899	-2.314	1.00	61.54
	1611	OH2	TIP	A	85	32.379	52.416	-8.311	1.00	71.84
	1612	OH2	TIP	A	86	48.425	50.638	14.271	1.00	59.92
	1613	OH2	TIP	A	87	10.680	67.805	5.635	1.00	55.82
	1614	OH2	TIP	A	88	36.880	58.553	1.670	1.00	57.31
	1615	OH2	TIP	A	89	16.870	52.214	1.693	1.00	58.45
	1616	OH2	TIP	A	90	25.408	92.634	4.035	1.00	58.03
	1617	OH2	TIP	A	91	13.095	80.378	22.328	1.00	50.36
	1618	OH2	TIP	A	92	29.763	48.629	0.935	1.00	57.19
	1619	OH2	TIP	A	93	48.144	52.717	5.484	1.00	62.27
	1620	OH2	TIP	A	94	32.716	83.953	9.514	1.00	61.49
	1621	OH2	TIP	A	95	50.245	51.781	10.104	1.00	66.72
	1622	OH2	TIP	A	96	19.486	103.622	14.976	1.00	62.93
	1623	OH2	TIP	A	97	16.771	101.927	12.421	1.00	59.08
	1624	OH2	TIP	A	98	53.390	55.312	11.504	1.00	66.54
	1625	OH2	TIP	A	99	50.837	51.731	13.291	1.00	64.16
	1626	OH2	TIP	A	100	23.981	65.804	-2.209	1.00	59.09
	1627	OH2	TIP	A	101	23.552	78.063	7.649	1.00	59.99
	1628	OH2	TIP	A	102	2.205	69.469	16.152	1.00	63.48
	1629	OH2	TIP	A	103	28.886	49.557	15.035	1.00	60.94
	1630	OH2	TIP	A	104	16.467	73.762	27.029	1.00	57.13
	1631	OH2	TIP	A	105	12.719	56.573	17.218	1.00	67.01
	1632	OH2	TIP	A	106	35.645	52.940	2.917	1.00	61.12
	1633	OH2	TIP	A	107	21.697	47.608	11.251	1.00	62.98
	1634	OH2	TIP	A	108	29.875	69.867	19.761	1.00	63.30
	1635	OH2	TIP	A	109	7.022	65.025	20.275	1.00	57.78
	1636	OH2	TIP	A	110	23.672	57.957	18.156	1.00	65.34
	1637	OH2	TIP	A	111	18.442	100.288	19.662	1.00	56.09
	1638	OH2	TIP	A	112	17.274	55.759	23.904	1.00	62.75
	1639	OH2	TIP	A	113	12.468	99.002	11.775	1.00	58.88
	1640	OH2	TIP	A	114	4.947	78.508	15.926	1.00	63.28
	1641	OH2	TIP	A	115	51.851	63.576	7.665	1.00	65.61
	1642	OH2	TIP	A	116	28.686	55.061	19.178	1.00	60.98
	1643	OH2	TIP	A	117	13.344	58.062	13.444	1.00	60.98
	1644	OH2	TIP	A	118	31.348	100.434	17.891	1.00	58.25
	1645	OH2	TIP	A	119	33.355	67.383	15.181	1.00	55.39
	1646	OH2	TIP	A	120	50.364	73.348	11.901	1.00	56.80
	1647	OH2	TIP	A	121	48.002	72.930	13.297	1.00	61.15
	1648	OH2	TIP	A	122	8.619	87.814	-3.671	1.00	55.82
	1649	OH2	TIP	A	123	28.580	65.220	7.059	1.00	45.14
	1650	OH2	TIP	A	124	17.490	63.562	13.375	1.00	55.49
	1651	OH2	TIP	A	125	50.105	70.842	12.277	1.00	66.22
	1652	OH2	TIP	A	126	28.516	67.863	5.456	1.00	57.00
	1653	OH2	TIP	A	127	7.299	75.901	18.432	1.00	57.60
	1654	OH2	TIP	A	128	16.230	56.580	0.876	1.00	56.82
	1655	OH2	TIP	A	129	29.715	52.741	21.104	1.00	62.05
	1656	OH2	TIP	A	130	46.391	75.590	10.503	1.00	66.31
	1657	OH2	TIP	A	131	8.623	74.686	21.869	1.00	57.71

	1658	OH2	TIP	A	132	25.877	65.684	-0.527	1.00	61.64
	1659	OH2	TIP	A	133	48.195	61.492	2.382	1.00	61.06
	1660	OH2	TIP	A	134	26.143	95.737	23.267	1.00	61.78
	1661	OH2	TIP	A	135	19.283	66.683	28.340	1.00	57.35
	1662	OH2	TIP	A	136	23.744	74.738	11.921	1.00	54.03
	1663	OH2	TIP	A	137	34.653	51.896	-6.794	1.00	64.00
	1664	OH2	TIP	A	138	23.762	64.741	24.873	1.00	65.85
	1665	OH2	TIP	A	139	9.472	67.784	26.691	1.00	60.91
	1666	OH2	TIP	A	140	31.126	79.895	13.795	1.00	61.62
	1667	OH2	TIP	A	141	51.302	75.595	10.454	1.00	62.13
	1668	OH2	TIP	A	142	25.624	94.976	18.923	1.00	58.14
	1669	OH2	TIP	A	143	46.215	76.102	4.024	1.00	61.05
	1670	OH2	TIP	A	144	14.705	65.280	31.014	1.00	55.65
	1671	OH2	TIP	A	145	39.069	49.876	20.322	1.00	64.64
	1672	OH2	TIP	A	146	10.862	54.941	15.417	1.00	61.54
	1673	OH2	TIP	A	147	20.183	101.944	22.268	1.00	59.07
	1674	OH2	TIP	A	148	29.707	89.335	8.858	1.00	60.79
	1675	OH2	TIP	A	149	10.193	73.823	5.510	1.00	57.59
	1676	OH2	TIP	A	150	29.352	51.313	-6.490	1.00	63.92
	1677	OH2	TIP	A	151	25.999	72.109	30.307	1.00	62.67
	1678	OH2	TIP	A	152	10.844	86.445	-4.018	1.00	68.07
	1679	OH2	TIP	A	153	30.550	70.355	12.969	1.00	61.87
	1680	OH2	TIP	A	154	28.953	49.265	12.349	1.00	66.95
	1681	OH2	TIP	A	155	10.816	50.012	8.484	1.00	59.56
	1682	OH2	TIP	A	156	27.343	69.536	30.284	1.00	59.20
	1683	OH2	TIP	A	157	48.276	50.311	10.430	1.00	67.18
	1684	OH2	TIP	A	158	9.916	67.356	2.963	1.00	59.37
	1685	OH2	TIP	A	159	24.834	107.006	22.307	1.00	65.79
	1686	OH2	TIP	A	160	15.746	59.001	13.607	1.00	58.89
	1687	OH2	TIP	A	161	31.698	74.365	32.777	1.00	59.68
	1688	OH2	TIP	A	162	21.890	56.335	-1.064	1.00	63.91
	1689	OH2	TIP	A	163	14.286	93.107	19.563	1.00	58.95
	1690	OH2	TIP	A	164	23.710	75.161	5.470	1.00	64.19
	1691	OH2	TIP	A	165	24.206	72.021	7.712	1.00	55.30
	1692	OH2	TIP	A	166	20.559	81.972	-0.663	1.00	55.04
	1693	OH2	TIP	A	167	28.070	68.574	17.772	1.00	61.56
	1694	OH2	TIP	A	168	57.914	63.409	6.737	1.00	63.55
	1695	OH2	TIP	A	169	18.340	57.211	25.770	1.00	62.46
	1696	OH2	TIP	A	170	26.782	106.710	18.895	1.00	61.28
	1697	OH2	TIP	A	171	28.254	75.284	31.745	1.00	59.15
	1698	OH2	TIP	A	172	46.877	48.708	12.388	1.00	66.69
	1699	OH2	TIP	A	173	15.777	67.027	-3.922	1.00	60.64
	1700	OH2	TIP	A	174	32.197	49.900	17.143	1.00	64.56
	1701	OH2	TIP	A	175	23.440	103.469	17.348	1.00	59.77
	1702	OH2	TIP	A	176	30.137	56.948	21.224	1.00	61.95
	1703	OH2	TIP	A	177	26.468	91.670	1.313	1.00	63.68
	1704	OH2	TIP	A	178	25.828	56.552	19.074	1.00	62.71
	1705	OH2	TIP	A	179	34.582	54.727	20.637	1.00	64.40
	1706	OH2	TIP	A	180	17.987	105.822	18.202	1.00	64.94
	1707	OH2	TIP	A	181	6.122	68.884	20.390	1.00	60.70
	1708	OH2	TIP	A	182	8.806	49.867	4.420	1.00	62.42
	1709	OH2	TIP	A	183	27.312	72.638	16.534	1.00	65.26
	1710	OH2	TIP	A	184	31.069	55.528	19.225	1.00	58.49
	1711	OH2	TIP	A	185	25.301	101.534	21.383	1.00	66.38
	1712	OH2	TIP	A	186	22.607	53.815	1.063	1.00	66.62
	1713	OH2	TIP	A	187	16.147	98.913	21.300	1.00	63.72
	1714	OH2	TIP	A	188	17.776	102.185	18.290	1.00	62.49
	1715	OH2	TIP	A	189	31.779	47.168	4.361	1.00	63.23
	1716	OH2	TIP	A	190	16.083	101.996	14.898	1.00	65.15
	1717	OH2	TIP	A	191	36.208	68.938	20.199	1.00	63.27
	1718	OH2	TIP	A	192	36.586	54.580	0.794	1.00	61.81
	1719	OH2	TIP	A	193	32.810	70.773	20.047	1.00	59.78

	1720	OH2	TIP	A	194	7.956	66.621	5.340	1.00	60.91
	1721	OH2	TIP	A	195	16.254	80.162	0.421	1.00	61.51
	1722	CB	VAL	B	336	45.054	59.383	30.496	1.00	63.58
	1723	CG1	VAL	B	336	45.744	60.010	31.695	1.00	64.78
	1724	CG2	VAL	B	336	44.712	57.923	30.765	1.00	68.51
	1725	C	VAL	B	336	44.164	61.555	29.666	1.00	61.62
	1726	O	VAL	B	336	45.201	61.720	29.026	1.00	64.02
	1727	N	VAL	B	336	42.976	59.439	29.128	1.00	59.58
	1728	CA	VAL	B	336	43.773	60.162	30.157	1.00	61.95
	1729	N	SER	B	337	43.338	62.554	29.963	1.00	59.54
	1730	CA	SER	B	337	43.618	63.921	29.536	1.00	57.94
	1731	CB	SER	B	337	42.531	64.396	28.575	1.00	56.70
	1732	OG	SER	B	337	41.253	64.019	29.047	1.00	65.28
	1733	C	SER	B	337	43.767	64.903	30.700	1.00	56.67
	1734	O	SER	B	337	43.366	64.613	31.832	1.00	56.61
	1735	N	ALA	B	338	44.355	66.061	30.413	1.00	52.92
	1736	CA	ALA	B	338	44.589	67.079	31.429	1.00	51.01
	1737	CB	ALA	B	338	46.038	67.024	31.884	1.00	50.96
	1738	C	ALA	B	338	44.252	68.480	30.934	1.00	50.95
	1739	O	ALA	B	338	44.396	68.784	29.748	1.00	53.16
	1740	N	TYR	B	339	43.795	69.328	31.850	1.00	47.68
	1741	CA	TYR	B	339	43.431	70.697	31.508	1.00	48.08
	1742	CB	TYR	B	339	41.925	70.790	31.203	1.00	50.34
	1743	CG	TYR	B	339	41.382	69.708	30.283	1.00	58.74
	1744	CD1	TYR	B	339	41.179	68.404	30.745	1.00	60.22
	1745	CE1	TYR	B	339	40.705	67.401	29.895	1.00	64.78
	1746	CD2	TYR	B	339	41.094	69.984	28.947	1.00	60.49
	1747	CE2	TYR	B	339	40.620	68.992	28.088	1.00	63.00
	1748	CZ	TYR	B	339	40.428	67.700	28.567	1.00	67.92
	1749	OH	TYR	B	339	39.974	66.709	27.718	1.00	68.47
	1750	C	TYR	B	339	43.785	71.646	32.663	1.00	45.49
	1751	O	TYR	B	339	43.556	71.338	33.833	1.00	43.52
	1752	N	LEU	B	340	44.362	72.792	32.325	1.00	44.01
	1753	CA	LEU	B	340	44.728	73.784	33.324	1.00	42.54
	1754	CB	LEU	B	340	46.237	74.050	33.284	1.00	39.07
	1755	CG	LEU	B	340	46.850	74.948	34.370	1.00	39.58
	1756	CD1	LEU	B	340	46.526	74.402	35.751	1.00	28.76
	1757	CD2	LEU	B	340	48.364	75.029	34.177	1.00	35.57
	1758	C	LEU	B	340	43.955	75.043	32.966	1.00	42.53
	1759	O	LEU	B	340	43.962	75.462	31.814	1.00	43.25
	1760	N	SER	B	341	43.276	75.643	33.940	1.00	42.42
	1761	CA	SER	B	341	42.497	76.848	33.675	1.00	40.32
	1762	CB	SER	B	341	41.014	76.603	33.995	1.00	41.30
	1763	OG	SER	B	341	40.842	76.184	35.336	1.00	45.86
	1764	C	SER	B	341	42.994	78.037	34.466	1.00	38.67
	1765	O	SER	B	341	43.552	77.893	35.541	1.00	42.94
	1766	N	ARG	B	342	42.777	79.222	33.923	1.00	37.60
	1767	CA	ARG	B	342	43.186	80.445	34.580	1.00	35.91
	1768	CB	ARG	B	342	43.241	81.574	33.548	1.00	36.67
	1769	CG	ARG	B	342	44.285	81.346	32.454	1.00	39.89
	1770	CD	ARG	B	342	44.278	82.459	31.421	1.00	42.31
	1771	NE	ARG	B	342	43.066	82.415	30.610	1.00	45.87
	1772	CZ	ARG	B	342	42.870	81.595	29.580	1.00	52.30
	1773	NH1	ARG	B	342	43.810	80.739	29.205	1.00	56.74
	1774	NH2	ARG	B	342	41.715	81.619	28.932	1.00	58.22
	1775	C	ARG	B	342	42.191	80.768	35.702	1.00	34.19
	1776	O	ARG	B	342	41.150	80.124	35.822	1.00	34.44
	1777	N	PRO	B	343	42.499	81.763	36.545	1.00	31.22
	1778	CD	PRO	B	343	43.729	82.572	36.606	1.00	34.08
	1779	CA	PRO	B	343	41.576	82.114	37.634	1.00	33.86
	1780	CB	PRO	B	343	42.356	83.163	38.437	1.00	32.10
	1781	CG	PRO	B	343	43.811	82.902	38.078	1.00	37.07

	1782	C	PRO	B	343	40.277	82.703	37.085	1.00	32.54
	1783	O	PRO	B	343	40.281	83.330	36.028	1.00	35.02
	1784	N	SER	B	344	39.168	82.510	37.789	1.00	33.04
	1785	CA	SER	B	344	37.913	83.085	37.322	1.00	34.74
	1786	CB	SER	B	344	36.703	82.428	38.005	1.00	35.18
	1787	OG	SER	B	344	36.507	82.937	39.308	1.00	35.70
	1788	C	SER	B	344	37.972	84.562	37.685	1.00	35.17
	1789	O	SER	B	344	38.468	84.931	38.751	1.00	32.53
	1790	N	PRO	B	345	37.506	85.438	36.787	1.00	35.98
	1791	CD	PRO	B	345	37.180	85.223	35.364	1.00	36.93
	1792	CA	PRO	B	345	37.544	86.869	37.105	1.00	34.79
	1793	CB	PRO	B	345	36.870	87.503	35.888	1.00	30.45
	1794	CG	PRO	B	345	37.379	86.612	34.769	1.00	30.91
	1795	C	PRO	B	345	36.861	87.215	38.433	1.00	34.13
	1796	O	PRO	B	345	37.283	88.129	39.137	1.00	34.14
	1797	N	PHE	B	346	35.817	86.476	38.791	1.00	31.57
	1798	CA	PHE	B	346	35.134	86.752	40.041	1.00	33.19
	1799	CB	PHE	B	346	33.876	85.889	40.165	1.00	37.49
	1800	CG	PHE	B	346	33.206	85.984	41.505	1.00	38.65
	1801	CD1	PHE	B	346	32.621	87.168	41.922	1.00	42.62
	1802	CD2	PHE	B	346	33.159	84.881	42.353	1.00	43.21
	1803	CE1	PHE	B	346	31.992	87.256	43.167	1.00	41.72
	1804	CE2	PHE	B	346	32.531	84.957	43.604	1.00	49.00
	1805	CZ	PHE	B	346	31.946	86.148	44.009	1.00	42.82
	1806	C	PHE	B	346	36.070	86.501	41.233	1.00	33.37
	1807	O	PHE	B	346	36.143	87.316	42.152	1.00	33.52
	1808	N	ASP	B	347	36.790	85.384	41.216	1.00	32.94
	1809	CA	ASP	B	347	37.709	85.067	42.308	1.00	33.61
	1810	CB	ASP	B	347	38.242	83.638	42.173	1.00	29.68
	1811	CG	ASP	B	347	37.222	82.589	42.559	1.00	35.85
	1812	OD1	ASP	B	347	37.516	81.386	42.382	1.00	42.71
	1813	OD2	ASP	B	347	36.128	82.954	43.044	1.00	50.58
	1814	C	ASP	B	347	38.882	86.036	42.338	1.00	33.62
	1815	O	ASP	B	347	39.381	86.399	43.401	1.00	30.10
	1816	N	LEU	B	348	39.312	86.463	41.160	1.00	34.23
	1817	CA	LEU	B	348	40.437	87.374	41.046	1.00	38.75
	1818	CB	LEU	B	348	40.964	87.340	39.604	1.00	38.06
	1819	CG	LEU	B	348	42.165	88.237	39.289	1.00	43.84
	1820	CD1	LEU	B	348	43.357	87.861	40.190	1.00	39.77
	1821	CD2	LEU	B	348	42.536	88.090	37.809	1.00	43.35
	1822	C	LEU	B	348	40.161	88.837	41.455	1.00	39.57
	1823	O	LEU	B	348	40.979	89.454	42.141	1.00	38.51
	1824	N	PHE	B	349	39.017	89.386	41.043	1.00	40.41
	1825	CA	PHE	B	349	38.699	90.791	41.338	1.00	42.87
	1826	CB	PHE	B	349	38.236	91.489	40.060	1.00	39.59
	1827	CG	PHE	B	349	39.217	91.392	38.937	1.00	37.95
	1828	CD1	PHE	B	349	38.951	90.596	37.832	1.00	36.40
	1829	CD2	PHE	B	349	40.419	92.083	38.995	1.00	40.49
	1830	CE1	PHE	B	349	39.874	90.484	36.795	1.00	39.63
	1831	CE2	PHE	B	349	41.353	91.981	37.965	1.00	38.12
	1832	CZ	PHE	B	349	41.080	91.182	36.863	1.00	41.86
	1833	C	PHE	B	349	37.704	91.128	42.446	1.00	44.67
	1834	O	PHE	B	349	37.827	92.167	43.099	1.00	47.25
	1835	N	ILE	B	350	36.705	90.286	42.650	1.00	46.06
	1836	CA	ILE	B	350	35.729	90.573	43.683	1.00	50.35
	1837	CB	ILE	B	350	34.330	90.052	43.287	1.00	50.30
	1838	CG2	ILE	B	350	33.284	90.603	44.236	1.00	51.91
	1839	CG1	ILE	B	350	34.007	90.454	41.839	1.00	51.78
	1840	CD1	ILE	B	350	34.234	91.915	41.520	1.00	45.73
	1841	C	ILE	B	350	36.179	89.906	44.973	1.00	51.95
	1842	O	ILE	B	350	36.454	90.572	45.970	1.00	52.71
	1843	N	ARG	B	351	36.281	88.584	44.927	1.00	53.39

	1844	CA	ARG	B	351	36.691	87.787	46.069	1.00	54.67
	1845	CB	ARG	B	351	36.541	86.310	45.707	1.00	59.14
	1846	CG	ARG	B	351	36.063	85.414	46.833	1.00	64.87
	1847	CD	ARG	B	351	35.127	84.346	46.292	1.00	66.51
	1848	NE	ARG	B	351	35.034	83.195	47.180	1.00	73.42
	1849	CZ	ARG	B	351	36.027	82.337	47.383	1.00	78.26
	1850	NH1	ARG	B	351	37.183	82.506	46.756	1.00	81.30
	1851	NH2	ARG	B	351	35.867	81.312	48.211	1.00	79.63
	1852	C	ARG	B	351	38.132	88.092	46.484	1.00	53.92
	1853	O	ARG	B	351	38.456	88.090	47.667	1.00	53.66
	1854	N	LYS	B	352	38.988	88.352	45.502	1.00	53.41
	1855	CA	LYS	B	352	40.400	88.658	45.740	1.00	53.02
	1856	CB	LYS	B	352	40.547	89.821	46.725	1.00	54.25
	1857	CG	LYS	B	352	39.848	91.094	46.286	1.00	64.61
	1858	CD	LYS	B	352	40.158	92.234	47.246	1.00	71.92
	1859	CE	LYS	B	352	39.190	93.398	47.086	1.00	76.75
	1860	NZ	LYS	B	352	37.807	93.027	47.505	1.00	82.42
	1861	C	LYS	B	352	41.217	87.470	46.253	1.00	51.14
	1862	O	LYS	B	352	42.183	87.655	46.991	1.00	51.55
	1863	N	SER	B	353	40.828	86.259	45.863	1.00	47.69
	1864	CA	SER	B	353	41.533	85.048	46.268	1.00	45.50
	1865	CB	SER	B	353	40.882	84.446	47.518	1.00	50.28
	1866	OG	SER	B	353	39.542	84.062	47.271	1.00	63.45
	1867	C	SER	B	353	41.465	84.072	45.094	1.00	40.39
	1868	O	SER	B	353	40.710	83.102	45.105	1.00	40.20
	1869	N	PRO	B	354	42.271	84.332	44.055	1.00	36.74
	1870	CD	PRO	B	354	43.262	85.412	44.061	1.00	36.52
	1871	CA	PRO	B	354	42.376	83.557	42.817	1.00	34.20
	1872	CB	PRO	B	354	43.283	84.418	41.937	1.00	31.70
	1873	CG	PRO	B	354	43.340	85.730	42.628	1.00	40.26
	1874	C	PRO	B	354	42.964	82.167	42.979	1.00	32.13
	1875	O	PRO	B	354	43.829	81.945	43.817	1.00	28.54
	1876	N	THR	B	355	42.489	81.241	42.158	1.00	30.96
	1877	CA	THR	B	355	42.999	79.882	42.164	1.00	31.86
	1878	CB	THR	B	355	42.099	78.908	42.979	1.00	32.67
	1879	OG1	THR	B	355	40.823	78.794	42.348	1.00	34.86
	1880	CG2	THR	B	355	41.894	79.406	44.401	1.00	34.90
	1881	C	THR	B	355	43.052	79.379	40.726	1.00	33.38
	1882	O	THR	B	355	42.361	79.897	39.840	1.00	32.61
	1883	N	ILE	B	356	43.909	78.403	40.482	1.00	32.83
	1884	CA	ILE	B	356	43.959	77.807	39.165	1.00	33.21
	1885	CB	ILE	B	356	45.297	78.062	38.434	1.00	34.88
	1886	CG2	ILE	B	356	45.458	79.562	38.190	1.00	34.84
	1887	CG1	ILE	B	356	46.465	77.502	39.240	1.00	37.26
	1888	CD1	ILE	B	356	47.843	77.791	38.611	1.00	38.06
	1889	C	ILE	B	356	43.745	76.335	39.461	1.00	32.48
	1890	O	ILE	B	356	44.037	75.861	40.564	1.00	30.30
	1891	N	THR	B	357	43.236	75.609	38.478	1.00	33.59
	1892	CA	THR	B	357	42.929	74.211	38.694	1.00	32.83
	1893	CB	THR	B	357	41.384	74.025	38.857	1.00	37.46
	1894	OG1	THR	B	357	40.955	74.615	40.091	1.00	35.11
	1895	CG2	THR	B	357	41.001	72.553	38.842	1.00	40.13
	1896	C	THR	B	357	43.420	73.326	37.570	1.00	34.22
	1897	O	THR	B	357	43.222	73.609	36.384	1.00	33.99
	1898	N	CYS	B	358	44.045	72.231	37.966	1.00	34.04
	1899	CA	CYS	B	358	44.563	71.256	37.032	1.00	36.90
	1900	C	CYS	B	358	43.573	70.104	37.101	1.00	36.26
	1901	O	CYS	B	358	43.412	69.497	38.156	1.00	35.68
	1902	CB	CYS	B	358	45.930	70.791	37.507	1.00	39.83
	1903	SG	CYS	B	358	46.881	69.819	36.302	1.00	52.73
	1904	N	LEU	B	359	42.908	69.820	35.988	1.00	38.57
	1905	CA	LEU	B	359	41.921	68.751	35.922	1.00	42.35

	1906	CB	LEU	B	359	40.615	69.273	35.304	1.00	42.11
40	1907	CG	LEU	B	359	39.572	68.227	34.881	1.00	48.42
	1908	CD1	LEU	B	359	39.146	67.379	36.073	1.00	49.46
	1909	CD2	LEU	B	359	38.370	68.934	34.269	1.00	48.09
	1910	C	LEU	B	359	42.437	67.589	35.095	1.00	45.39
	1911	O	LEU	B	359	42.794	67.766	33.935	1.00	48.73
45	1912	N	VAL	B	360	42.479	66.405	35.693	1.00	47.72
	1913	CA	VAL	B	360	42.931	65.205	34.996	1.00	51.87
	1914	CB	VAL	B	360	44.075	64.514	35.765	1.00	52.99
	1915	CG1	VAL	B	360	44.490	63.235	35.051	1.00	51.29
	1916	CG2	VAL	B	360	45.252	65.456	35.890	1.00	52.42
50	1917	C	VAL	B	360	41.767	64.221	34.874	1.00	55.21
	1918	O	VAL	B	360	41.063	63.966	35.853	1.00	56.01
	1919	N	VAL	B	361	41.558	63.680	33.677	1.00	57.47
	1920	CA	VAL	B	361	40.479	62.718	33.448	1.00	61.75
	1921	CB	VAL	B	361	39.447	63.248	32.425	1.00	58.91
55	1922	CG1	VAL	B	361	38.368	62.211	32.187	1.00	56.98
	1923	CG2	VAL	B	361	38.826	64.530	32.934	1.00	54.49
	1924	C	VAL	B	361	41.045	61.403	32.923	1.00	66.78
	1925	O	VAL	B	361	41.836	61.392	31.981	1.00	67.30
	1926	N	ASP	B	362	40.641	60.299	33.544	1.00	72.35
5	1927	CA	ASP	B	362	41.100	58.969	33.145	1.00	79.16
	1928	CB	ASP	B	362	41.775	58.266	34.331	1.00	83.66
	1929	CG	ASP	B	362	42.511	56.997	33.924	1.00	87.40
	1930	OD1	ASP	B	362	42.317	56.529	32.780	1.00	91.40
	1931	OD2	ASP	B	362	43.282	56.462	34.752	1.00	87.33
10	1932	C	ASP	B	362	39.896	58.156	32.676	1.00	82.84
	1933	O	ASP	B	362	39.113	57.663	33.493	1.00	84.14
	1934	N	ALA	B	363	39.751	58.022	31.360	1.00	85.70
	1935	CA	ALA	B	363	38.636	57.281	30.775	1.00	89.05
	1936	CB	ALA	B	363	38.830	57.154	29.270	1.00	90.18
15	1937	C	ALA	B	363	38.458	55.899	31.401	1.00	91.80
	1938	O	ALA	B	363	37.354	55.357	31.409	1.00	92.23
	1939	N	ALA	B	364	39.544	55.337	31.926	1.00	94.23
	1940	CA	ALA	B	364	39.515	54.022	32.564	1.00	97.42
	1941	CB	ALA	B	364	39.441	52.932	31.506	1.00	96.05
20	1942	C	ALA	B	364	40.772	53.845	33.413	1.00	100.00
	1943	O	ALA	B	364	41.885	53.833	32.887	1.00	101.29
	1944	N	PRO	B	365	40.612	53.715	34.741	1.00	101.76
	1945	CD	PRO	B	365	39.442	54.193	35.503	1.00	101.62
	1946	CA	PRO	B	365	41.764	53.547	35.632	1.00	103.14
25	1947	CB	PRO	B	365	41.486	54.578	36.706	1.00	103.27
	1948	CG	PRO	B	365	40.006	54.372	36.917	1.00	103.12
	1949	C	PRO	B	365	41.919	52.144	36.228	1.00	104.03
	1950	O	PRO	B	365	42.228	51.181	35.521	1.00	104.47
	1951	N	ALA	B	366	41.716	52.064	37.543	1.00	104.37
30	1952	CA	ALA	B	366	41.807	50.824	38.307	1.00	104.87
	1953	CB	ALA	B	366	40.895	49.761	37.687	1.00	105.36
	1954	C	ALA	B	366	43.230	50.281	38.435	1.00	104.90
	1955	O	ALA	B	366	43.492	49.139	38.055	1.00	105.14
	1956	N	LYS	B	367	44.148	51.086	38.971	1.00	104.05
35	1957	CA	LYS	B	367	45.523	50.618	39.128	1.00	103.07
	1958	CB	LYS	B	367	46.061	50.117	37.785	1.00	103.33
	1959	CG	LYS	B	367	46.194	51.189	36.717	1.00	102.12
	1960	CD	LYS	B	367	46.962	50.649	35.528	1.00	103.99
	1961	CE	LYS	B	367	47.229	51.724	34.496	1.00	103.83
40	1962	NZ	LYS	B	367	48.056	51.183	33.386	1.00	105.88
	1963	C	LYS	B	367	46.554	51.576	39.727	1.00	102.12
	1964	O	LYS	B	367	47.653	51.712	39.185	1.00	103.05
	1965	N	GLY	B	368	46.228	52.235	40.835	1.00	99.91
	1966	CA	GLY	B	368	47.212	53.120	41.436	1.00	96.70
45	1967	C	GLY	B	368	46.800	54.521	41.845	1.00	94.03

	1968	O	GLY	B	368	45.651	54.771	42.209	1.00	94.76
	1969	N	ALA	B	369	47.761	55.438	41.787	1.00	90.44
	1970	CA	ALA	B	369	47.534	56.828	42.165	1.00	86.18
	1971	CB	ALA	B	369	48.292	57.140	43.455	1.00	86.97
	1972	C	ALA	B	369	47.961	57.792	41.062	1.00	82.79
	1973	O	ALA	B	369	48.773	57.451	40.203	1.00	83.46
	1974	N	VAL	B	370	47.407	59.000	41.099	1.00	78.82
	1975	CA	VAL	B	370	47.719	60.033	40.115	1.00	73.44
	1976	CB	VAL	B	370	46.468	60.439	39.323	1.00	71.37
	1977	CG1	VAL	B	370	46.837	61.455	38.260	1.00	68.72
	1978	CG2	VAL	B	370	45.831	59.212	38.696	1.00	66.32
	1979	C	VAL	B	370	48.254	61.253	40.848	1.00	71.19
	1980	O	VAL	B	370	47.581	61.797	41.717	1.00	70.77
	1981	N	ASN	B	371	49.462	61.687	40.495	1.00	69.11
	1982	CA	ASN	B	371	50.069	62.831	41.164	1.00	67.35
	1983	CB	ASN	B	371	51.462	62.455	41.670	1.00	68.95
	1984	CG	ASN	B	371	51.432	61.270	42.602	1.00	73.37
	1985	OD1	ASN	B	371	50.772	61.301	43.641	1.00	76.52
	1986	ND2	ASN	B	371	52.146	60.213	42.237	1.00	76.06
	1987	C	ASN	B	371	50.159	64.109	40.334	1.00	65.35
	1988	O	ASN	B	371	50.454	64.084	39.136	1.00	63.63
	1989	N	LEU	B	372	49.892	65.227	41.000	1.00	63.51
	1990	CA	LEU	B	372	49.949	66.540	40.379	1.00	60.50
	1991	CB	LEU	B	372	48.573	67.214	40.395	1.00	60.09
	1992	CG	LEU	B	372	47.430	66.461	39.714	1.00	61.37
	1993	CD1	LEU	B	372	46.196	67.335	39.688	1.00	63.12
	1994	CD2	LEU	B	372	47.829	66.083	38.309	1.00	62.53
	1995	C	LEU	B	372	50.942	67.380	41.164	1.00	57.54
	1996	O	LEU	B	372	50.824	67.531	42.380	1.00	58.06
	1997	N	THR	B	373	51.926	67.919	40.458	1.00	54.64
	1998	CA	THR	B	373	52.952	68.745	41.074	1.00	52.59
	1999	CB	THR	B	373	54.346	68.175	40.786	1.00	54.37
	2000	OG1	THR	B	373	54.383	66.801	41.191	1.00	60.15
	2001	CG2	THR	B	373	55.409	68.955	41.545	1.00	57.66
	2002	C	THR	B	373	52.878	70.156	40.509	1.00	48.12
	2003	O	THR	B	373	52.803	70.337	39.297	1.00	46.78
	2004	N	TRP	B	374	52.895	71.150	41.391	1.00	45.42
	2005	CA	TRP	B	374	52.833	72.543	40.971	1.00	44.33
	2006	CB	TRP	B	374	51.838	73.340	41.823	1.00	40.42
	2007	CG	TRP	B	374	50.417	72.936	41.658	1.00	41.22
	2008	CD2	TRP	B	374	49.510	73.385	40.643	1.00	35.68
	2009	CE2	TRP	B	374	48.271	72.759	40.881	1.00	31.67
	2010	CE3	TRP	B	374	49.628	74.258	39.555	1.00	35.08
	2011	CD1	TRP	B	374	49.712	72.077	42.448	1.00	38.77
	2012	NE1	TRP	B	374	48.420	71.966	41.988	1.00	37.27
	2013	CZ2	TRP	B	374	47.153	72.979	40.073	1.00	32.53
	2014	CZ3	TRP	B	374	48.516	74.479	38.748	1.00	36.03
	2015	CH2	TRP	B	374	47.296	73.840	39.013	1.00	33.34
	2016	C	TRP	B	374	54.195	73.215	41.078	1.00	44.84
	2017	O	TRP	B	374	55.019	72.842	41.914	1.00	43.54
	2018	N	SER	B	375	54.419	74.205	40.218	1.00	44.41
	2019	CA	SER	B	375	55.660	74.967	40.213	1.00	45.63
	2020	CB	SER	B	375	56.800	74.168	39.565	1.00	47.59
	2021	OG	SER	B	375	56.662	74.088	38.157	1.00	49.42
	2022	C	SER	B	375	55.488	76.292	39.482	1.00	45.23
	2023	O	SER	B	375	54.609	76.438	38.629	1.00	46.27
	2024	N	ARG	B	376	56.323	77.259	39.843	1.00	42.63
	2025	CA	ARG	B	376	56.293	78.567	39.218	1.00	41.96
	2026	CB	ARG	B	376	56.337	79.676	40.266	1.00	43.72
	2027	CG	ARG	B	376	55.142	79.745	41.199	1.00	40.62
	2028	CD	ARG	B	376	54.907	81.195	41.580	1.00	41.72
	2029	NE	ARG	B	376	55.132	81.457	42.990	1.00	52.53

	2030	CZ	ARG	B	376	55.295	82.671	43.501	1.00	52.81
	2031	NH1	ARG	B	376	55.265	83.741	42.714	1.00	51.46
55	2032	NH2	ARG	B	376	55.472	82.819	44.807	1.00	56.61
	2033	C	ARG	B	376	57.518	78.680	38.325	1.00	39.96
	2034	O	ARG	B	376	58.629	78.382	38.745	1.00	40.84
	2035	N	ALA	B	377	57.315	79.097	37.086	1.00	41.64
	2036	CA	ALA	B	377	58.423	79.250	36.154	1.00	41.34
5	2037	CB	ALA	B	377	57.920	79.895	34.873	1.00	33.50
	2038	C	ALA	B	377	59.544	80.098	36.775	1.00	41.22
	2039	O	ALA	B	377	60.712	79.915	36.452	1.00	41.04
	2040	N	SER	B	378	59.179	81.008	37.677	1.00	40.92
	2041	CA	SER	B	378	60.149	81.881	38.327	1.00	42.71
10	2042	CB	SER	B	378	59.461	83.109	38.915	1.00	44.29
	2043	OG	SER	B	378	58.733	82.758	40.080	1.00	42.78
	2044	C	SER	B	378	60.894	81.180	39.442	1.00	43.58
	2045	O	SER	B	378	61.809	81.749	40.022	1.00	44.22
	2046	N	GLY	B	379	60.483	79.954	39.751	1.00	43.82
15	2047	CA	GLY	B	379	61.137	79.191	40.796	1.00	45.23
	2048	C	GLY	B	379	60.683	79.540	42.199	1.00	48.43
	2049	O	GLY	B	379	61.038	78.853	43.157	1.00	47.67
	2050	N	LYS	B	380	59.901	80.605	42.337	1.00	50.04
	2051	CA	LYS	B	380	59.423	80.997	43.653	1.00	52.22
20	2052	CB	LYS	B	380	58.732	82.362	43.591	1.00	54.82
	2053	CG	LYS	B	380	59.721	83.504	43.454	1.00	63.15
	2054	CD	LYS	B	380	59.072	84.866	43.634	1.00	70.67
	2055	CE	LYS	B	380	60.133	85.960	43.645	1.00	75.50
	2056	NZ	LYS	B	380	59.549	87.325	43.746	1.00	80.58
25	2057	C	LYS	B	380	58.493	79.945	44.249	1.00	52.26
	2058	O	LYS	B	380	57.944	79.105	43.535	1.00	49.96
	2059	N	PRO	B	381	58.315	79.974	45.578	1.00	53.55
	2060	CD	PRO	B	381	58.943	80.906	46.529	1.00	54.43
	2061	CA	PRO	B	381	57.453	79.016	46.282	1.00	54.97
30	2062	CB	PRO	B	381	57.652	79.388	47.755	1.00	57.06
	2063	CG	PRO	B	381	58.989	80.081	47.773	1.00	59.10
	2064	C	PRO	B	381	55.974	79.068	45.893	1.00	54.14
	2065	O	PRO	B	381	55.422	80.143	45.633	1.00	55.04
	2066	N	VAL	B	382	55.344	77.899	45.849	1.00	52.78
35	2067	CA	VAL	B	382	53.920	77.799	45.554	1.00	53.97
	2068	CB	VAL	B	382	53.603	76.709	44.489	1.00	54.50
	2069	CG1	VAL	B	382	54.348	77.005	43.204	1.00	56.74
	2070	CG2	VAL	B	382	53.955	75.319	45.022	1.00	46.72
	2071	C	VAL	B	382	53.262	77.398	46.874	1.00	54.10
40	2072	O	VAL	B	382	53.865	76.690	47.683	1.00	53.38
	2073	N	ASN	B	383	52.034	77.848	47.089	1.00	53.55
	2074	CA	ASN	B	383	51.311	77.527	48.310	1.00	54.35
	2075	CB	ASN	B	383	50.115	78.465	48.470	1.00	60.43
	2076	CG	ASN	B	383	50.513	79.923	48.471	1.00	67.43
45	2077	OD1	ASN	B	383	49.710	80.794	48.137	1.00	75.26
	2078	ND2	ASN	B	383	51.755	80.201	48.856	1.00	72.99
	2079	C	ASN	B	383	50.822	76.080	48.318	1.00	52.64
	2080	O	ASN	B	383	51.082	75.308	47.393	1.00	50.26
	2081	N	HIS	B	384	50.107	75.721	49.376	1.00	51.74
50	2082	CA	HIS	B	384	49.562	74.375	49.515	1.00	51.28
	2083	CB	HIS	B	384	49.220	74.101	50.979	1.00	59.06
	2084	CG	HIS	B	384	50.421	73.943	51.861	1.00	65.42
	2085	CD2	HIS	B	384	50.873	74.688	52.896	1.00	72.26
	2086	ND1	HIS	B	384	51.316	72.906	51.715	1.00	70.87
55	2087	CE1	HIS	B	384	52.270	73.019	52.623	1.00	76.58

	2088	NE2	HIS	B	384	52.024	74.093	53.353	1.00	77.95
	2089	C	HIS	B	384	48.306	74.238	48.655	1.00	47.99
	2090	O	HIS	B	384	47.455	75.122	48.644	1.00	45.37
	2091	N	SER	B	385	48.187	73.127	47.944	1.00	45.57
	2092	CA	SER	B	385	47.036	72.926	47.085	1.00	45.69
	2093	CB	SER	B	385	47.503	72.466	45.695	1.00	41.19
	2094	OG	SER	B	385	48.315	71.301	45.762	1.00	41.34
	2095	C	SER	B	385	46.002	71.946	47.660	1.00	44.94
	2096	O	SER	B	385	46.287	71.187	48.582	1.00	41.64
	2097	N	THR	B	386	44.795	71.997	47.107	1.00	45.73
	2098	CA	THR	B	386	43.702	71.133	47.521	1.00	46.08
	2099	CB	THR	B	386	42.409	71.930	47.737	1.00	47.42
	2100	OG1	THR	B	386	42.576	72.825	48.844	1.00	50.45
	2101	CG2	THR	B	386	41.253	70.985	48.025	1.00	51.73
	2102	C	THR	B	386	43.468	70.113	46.419	1.00	46.45
	2103	O	THR	B	386	43.359	70.471	45.247	1.00	47.06
	2104	N	ARG	B	387	43.394	68.846	46.808	1.00	46.33
	2105	CA	ARG	B	387	43.190	67.751	45.872	1.00	46.50
	2106	CB	ARG	B	387	44.310	66.726	46.070	1.00	48.08
	2107	CG	ARG	B	387	44.234	65.514	45.167	1.00	54.89
	2108	CD	ARG	B	387	45.119	64.392	45.695	1.00	59.67
	2109	NE	ARG	B	387	44.932	63.162	44.935	1.00	63.12
	2110	CZ	ARG	B	387	45.650	62.825	43.870	1.00	65.65
	2111	NH1	ARG	B	387	46.618	63.629	43.449	1.00	67.29
	2112	NH2	ARG	B	387	45.385	61.701	43.211	1.00	63.40
	2113	C	ARG	B	387	41.814	67.083	46.054	1.00	46.30
	2114	O	ARG	B	387	41.361	66.867	47.179	1.00	44.30
	2115	N	LYS	B	388	41.159	66.766	44.938	1.00	45.70
	2116	CA	LYS	B	388	39.851	66.111	44.960	1.00	44.68
	2117	CB	LYS	B	388	38.748	67.121	44.634	1.00	46.84
	2118	CG	LYS	B	388	38.669	68.263	45.624	1.00	56.94
	2119	CD	LYS	B	388	37.921	69.450	45.046	1.00	58.62
	2120	CE	LYS	B	388	38.293	70.717	45.791	1.00	61.92
	2121	NZ	LYS	B	388	37.744	71.924	45.123	1.00	70.07
	2122	C	LYS	B	388	39.802	64.954	43.957	1.00	44.52
	2123	O	LYS	B	388	40.221	65.098	42.806	1.00	40.60
	2124	N	GLU	B	389	39.296	63.807	44.411	1.00	47.26
	2125	CA	GLU	B	389	39.176	62.599	43.582	1.00	50.72
	2126	CB	GLU	B	389	40.069	61.486	44.135	1.00	54.88
	2127	CG	GLU	B	389	41.559	61.752	44.061	1.00	67.37
	2128	CD	GLU	B	389	42.375	60.621	44.664	1.00	75.83
	2129	OE1	GLU	B	389	41.858	59.484	44.736	1.00	79.33
	2130	OE2	GLU	B	389	43.538	60.862	45.056	1.00	80.70
	2131	C	GLU	B	389	37.729	62.090	43.549	1.00	51.11
	2132	O	GLU	B	389	37.090	61.956	44.596	1.00	48.28
	2133	N	ALA	B	390	37.218	61.786	42.359	1.00	52.07
	2134	CA	ALA	B	390	35.845	61.303	42.232	1.00	56.84
	2135	CB	ALA	B	390	34.888	62.480	42.128	1.00	53.86
	2136	C	ALA	B	390	35.643	60.371	41.042	1.00	60.96
	2137	O	ALA	B	390	36.285	60.515	40.002	1.00	61.14
	2138	N	ALA	B	391	34.727	59.421	41.204	1.00	65.61
	2139	CA	ALA	B	391	34.413	58.449	40.162	1.00	68.46
	2140	CB	ALA	B	391	35.264	57.202	40.339	1.00	71.73
	2141	C	ALA	B	391	32.939	58.082	40.234	1.00	70.37
	2142	O	ALA	B	391	32.139	58.524	39.412	1.00	72.17
	2143	N	LEU	B	397	37.390	58.285	36.020	1.00	60.70
	2144	CA	LEU	B	397	37.949	58.914	37.210	1.00	61.36
	2145	CB	LEU	B	397	39.142	58.111	37.725	1.00	64.28
	2146	CG	LEU	B	397	39.864	58.746	38.920	1.00	65.19
	2147	CD1	LEU	B	397	38.930	58.798	40.119	1.00	65.40
	2148	CD2	LEU	B	397	41.115	57.948	39.256	1.00	68.57
	2149	C	LEU	B	397	38.389	60.359	36.981	1.00	61.24

	2150	O	LEU	B	397	39.115	60.666	36.036	1.00	62.11
	2151	N	THR	B	398	37.946	61.240	37.867	1.00	59.83
	2152	CA	THR	B	398	38.291	62.650	37.795	1.00	58.04
	2153	CB	THR	B	398	37.028	63.539	37.837	1.00	58.72
	2154	OG1	THR	B	398	36.322	63.429	36.594	1.00	64.28
	2155	CG2	THR	B	398	37.403	64.992	38.077	1.00	61.55
	2156	C	THR	B	398	39.199	63.027	38.965	1.00	55.72
	2157	O	THR	B	398	39.005	62.579	40.100	1.00	55.02
	2158	N	VAL	B	399	40.199	63.848	38.678	1.00	52.38
	2159	CA	VAL	B	399	41.127	64.303	39.698	1.00	49.13
	2160	CB	VAL	B	399	42.421	63.457	39.709	1.00	51.57
	2161	CG1	VAL	B	399	43.388	64.006	40.737	1.00	52.00
	2162	CG2	VAL	B	399	42.100	62.010	40.032	1.00	55.81
	2163	C	VAL	B	399	41.507	65.753	39.457	1.00	46.27
	2164	O	VAL	B	399	41.951	66.122	38.368	1.00	43.17
	2165	N	THR	B	400	41.311	66.585	40.470	1.00	44.56
	2166	CA	THR	B	400	41.685	67.981	40.342	1.00	43.39
	2167	CB	THR	B	400	40.460	68.931	40.271	1.00	41.43
	2168	OG1	THR	B	400	39.806	68.972	41.543	1.00	48.65
	2169	CG2	THR	B	400	39.480	68.474	39.211	1.00	38.93
	2170	C	THR	B	400	42.541	68.426	41.516	1.00	40.85
	2171	O	THR	B	400	42.506	67.849	42.606	1.00	35.85
	2172	N	SER	B	401	43.333	69.454	41.253	1.00	39.13
	2173	CA	SER	B	401	44.183	70.058	42.253	1.00	37.93
	2174	CB	SER	B	401	45.656	69.715	42.021	1.00	40.15
	2175	OG	SER	B	401	46.458	70.310	43.031	1.00	44.51
	2176	C	SER	B	401	43.978	71.546	42.056	1.00	36.16
	2177	O	SER	B	401	44.139	72.048	40.947	1.00	36.19
	2178	N	THR	B	402	43.611	72.238	43.125	1.00	32.94
	2179	CA	THR	B	402	43.396	73.669	43.061	1.00	32.35
	2180	CB	THR	B	402	42.022	74.022	43.617	1.00	33.13
	2181	OG1	THR	B	402	41.041	73.321	42.854	1.00	34.46
	2182	CG2	THR	B	402	41.755	75.514	43.523	1.00	33.71
	2183	C	THR	B	402	44.483	74.378	43.857	1.00	31.66
	2184	O	THR	B	402	44.714	74.088	45.036	1.00	26.99
	2185	N	LEU	B	403	45.141	75.318	43.187	1.00	32.16
	2186	CA	LEU	B	403	46.230	76.074	43.781	1.00	32.46
	2187	CB	LEU	B	403	47.477	75.952	42.895	1.00	34.12
	2188	CG	LEU	B	403	48.762	76.680	43.306	1.00	34.78
	2189	CD1	LEU	B	403	49.404	75.922	44.456	1.00	35.87
	2190	CD2	LEU	B	403	49.727	76.744	42.132	1.00	31.42
	2191	C	LEU	B	403	45.910	77.548	44.001	1.00	33.39
	2192	O	LEU	B	403	45.595	78.279	43.060	1.00	30.14
	2193	N	PRO	B	404	45.967	77.996	45.265	1.00	34.13
	2194	CD	PRO	B	404	46.187	77.209	46.495	1.00	34.29
	2195	CA	PRO	B	404	45.701	79.397	45.587	1.00	34.91
	2196	CB	PRO	B	404	45.823	79.439	47.108	1.00	33.92
	2197	CG	PRO	B	404	45.479	78.046	47.526	1.00	33.77
	2198	C	PRO	B	404	46.827	80.173	44.909	1.00	36.43
	2199	O	PRO	B	404	47.990	79.776	44.960	1.00	30.87
	2200	N	VAL	B	405	46.480	81.274	44.265	1.00	37.52
	2201	CA	VAL	B	405	47.471	82.068	43.569	1.00	41.37
	2202	CB	VAL	B	405	47.138	82.078	42.047	1.00	44.39
	2203	CG1	VAL	B	405	47.034	83.500	41.513	1.00	47.81
	2204	CG2	VAL	B	405	48.180	81.288	41.301	1.00	43.63
	2205	C	VAL	B	405	47.544	83.492	44.120	1.00	42.93
	2206	O	VAL	B	405	46.553	84.042	44.589	1.00	42.10
	2207	N	GLY	B	406	48.732	84.082	44.081	1.00	45.32
	2208	CA	GLY	B	406	48.869	85.446	44.553	1.00	46.40
	2209	C	GLY	B	406	48.208	86.373	43.548	1.00	46.70
	2210	O	GLY	B	406	48.345	86.179	42.334	1.00	41.89
	2211	N	THR	B	407	47.486	87.373	44.052	1.00	46.37

	2212	CA	THR	B	407	46.791	88.341	43.208	1.00	49.05
	2213	CB	THR	B	407	45.983	89.348	44.062	1.00	51.01
	2214	OG1	THR	B	407	44.900	88.671	44.709	1.00	55.76
	2215	CG2	THR	B	407	45.423	90.453	43.195	1.00	54.66
	2216	C	THR	B	407	47.746	89.132	42.325	1.00	49.24
	2217	O	THR	B	407	47.597	89.154	41.105	1.00	48.91
	2218	N	ALA	B	408	48.726	89.777	42.953	1.00	49.71
	2219	CA	ALA	B	408	49.693	90.592	42.240	1.00	50.13
	2220	CB	ALA	B	408	50.562	91.367	43.224	1.00	53.74
	2221	C	ALA	B	408	50.569	89.777	41.312	1.00	51.25
	2222	O	ALA	B	408	50.852	90.207	40.191	1.00	50.28
	2223	N	ASP	B	409	51.000	88.605	41.770	1.00	50.74
	2224	CA	ASP	B	409	51.852	87.748	40.948	1.00	52.13
	2225	CB	ASP	B	409	52.265	86.498	41.730	1.00	58.27
	2226	CG	ASP	B	409	53.065	86.830	42.977	1.00	69.38
	2227	OD1	ASP	B	409	54.121	87.495	42.848	1.00	75.94
	2228	OD2	ASP	B	409	52.641	86.431	44.084	1.00	72.00
	2229	C	ASP	B	409	51.151	87.341	39.655	1.00	49.96
	2230	O	ASP	B	409	51.769	87.283	38.588	1.00	49.48
	2231	N	TRP	B	410	49.858	87.058	39.755	1.00	46.74
	2232	CA	TRP	B	410	49.106	86.669	38.583	1.00	44.75
	2233	CB	TRP	B	410	47.732	86.113	38.957	1.00	39.75
	2234	CG	TRP	B	410	46.999	85.687	37.738	1.00	37.35
	2235	CD2	TRP	B	410	47.191	84.469	37.017	1.00	31.03
	2236	CE2	TRP	B	410	46.412	84.551	35.846	1.00	29.68
	2237	CE3	TRP	B	410	47.963	83.314	37.243	1.00	32.46
	2238	CD1	TRP	B	410	46.119	86.434	37.001	1.00	32.61
	2239	NE1	TRP	B	410	45.767	85.758	35.868	1.00	33.45
	2240	CZ2	TRP	B	410	46.370	83.522	34.900	1.00	29.11
	2241	CZ3	TRP	B	410	47.920	82.290	36.302	1.00	34.12
	2242	CH2	TRP	B	410	47.128	82.405	35.142	1.00	35.80
	2243	C	TRP	B	410	48.934	87.857	37.649	1.00	43.08
	2244	O	TRP	B	410	49.137	87.733	36.445	1.00	38.95
	2245	N	ILE	B	411	48.563	89.007	38.206	1.00	46.39
	2246	CA	ILE	B	411	48.372	90.211	37.404	1.00	51.22
	2247	CB	ILE	B	411	47.848	91.382	38.259	1.00	53.02
	2248	CG2	ILE	B	411	47.705	92.628	37.401	1.00	55.27
	2249	CG1	ILE	B	411	46.488	91.010	38.860	1.00	56.63
	2250	CD1	ILE	B	411	45.858	92.102	39.733	1.00	61.16
	2251	C	ILE	B	411	49.669	90.632	36.729	1.00	52.33
	2252	O	ILE	B	411	49.645	91.196	35.638	1.00	53.32
	2253	N	GLU	B	412	50.800	90.333	37.369	1.00	54.18
	2254	CA	GLU	B	412	52.099	90.693	36.821	1.00	53.56
	2255	CB	GLU	B	412	53.110	90.908	37.942	1.00	58.95
	2256	CG	GLU	B	412	53.034	92.302	38.528	1.00	73.61
	2257	CD	GLU	B	412	54.062	92.542	39.612	1.00	83.01
	2258	OE1	GLU	B	412	55.244	92.185	39.411	1.00	89.18
	2259	OE2	GLU	B	412	53.691	93.102	40.665	1.00	89.24
	2260	C	GLU	B	412	52.665	89.726	35.793	1.00	51.42
	2261	O	GLU	B	412	53.725	89.985	35.227	1.00	50.68
	2262	N	GLY	B	413	51.967	88.617	35.551	1.00	48.27
	2263	CA	GLY	B	413	52.428	87.671	34.551	1.00	46.15
	2264	C	GLY	B	413	53.111	86.377	34.967	1.00	44.58
	2265	O	GLY	B	413	53.637	85.675	34.106	1.00	42.91
	2266	N	GLU	B	414	53.118	86.044	36.256	1.00	44.06
	2267	CA	GLU	B	414	53.749	84.799	36.685	1.00	42.21
	2268	CB	GLU	B	414	53.467	84.523	38.172	1.00	42.27
	2269	CG	GLU	B	414	53.963	83.159	38.698	1.00	44.30
	2270	CD	GLU	B	414	55.487	83.036	38.739	1.00	52.18
	2271	OE1	GLU	B	414	56.083	82.562	37.745	1.00	51.39
	2272	OE2	GLU	B	414	56.090	83.425	39.764	1.00	49.53
	2273	C	GLU	B	414	53.147	83.690	35.839	1.00	41.40

	2274	O	GLU	B	414	51.995	83.781	35.413	1.00	38.41
	2275	N	THR	B	415	53.936	82.656	35.573	1.00	41.90
	2276	CA	THR	B	415	53.454	81.522	34.806	1.00	43.26
	2277	CB	THR	B	415	54.281	81.341	33.506	1.00	46.09
	2278	OG1	THR	B	415	54.155	79.996	33.032	1.00	50.78
	2279	CG2	THR	B	415	55.716	81.690	33.734	1.00	56.55
	2280	C	THR	B	415	53.499	80.270	35.690	1.00	41.87
	2281	O	THR	B	415	54.533	79.963	36.285	1.00	43.61
	2282	N	TYR	B	416	52.371	79.571	35.806	1.00	39.27
	2283	CA	TYR	B	416	52.309	78.378	36.650	1.00	37.37
	2284	CB	TYR	B	416	51.102	78.428	37.581	1.00	33.61
	2285	CG	TYR	B	416	51.064	79.633	38.478	1.00	27.57
	2286	CD1	TYR	B	416	50.753	80.894	37.974	1.00	26.31
	2287	CE1	TYR	B	416	50.752	82.009	38.800	1.00	35.08
	2288	CD2	TYR	B	416	51.371	79.516	39.825	1.00	28.68
	2289	CE2	TYR	B	416	51.379	80.615	40.651	1.00	30.56
	2290	CZ	TYR	B	416	51.070	81.857	40.140	1.00	35.62
	2291	OH	TYR	B	416	51.088	82.944	40.984	1.00	44.94
	2292	C	TYR	B	416	52.256	77.106	35.833	1.00	38.31
	2293	O	TYR	B	416	51.744	77.092	34.709	1.00	37.29
	2294	N	GLN	B	417	52.781	76.031	36.416	1.00	39.74
	2295	CA	GLN	B	417	52.823	74.751	35.736	1.00	40.75
	2296	CB	GLN	B	417	54.254	74.457	35.264	1.00	41.60
	2297	CG	GLN	B	417	54.353	73.240	34.349	1.00	53.57
	2298	CD	GLN	B	417	55.762	72.997	33.829	1.00	65.04
	2299	OE1	GLN	B	417	56.481	72.124	34.325	1.00	69.74
	2300	NE2	GLN	B	417	56.165	73.777	32.831	1.00	66.91
	2301	C	GLN	B	417	52.320	73.578	36.565	1.00	39.48
	2302	O	GLN	B	417	52.619	73.451	37.754	1.00	40.03
	2303	N	CYS	B	418	51.557	72.718	35.912	1.00	39.47
	2304	CA	CYS	B	418	51.032	71.525	36.541	1.00	41.39
	2305	C	CYS	B	418	51.732	70.354	35.868	1.00	41.00
	2306	O	CYS	B	418	51.661	70.205	34.648	1.00	41.94
	2307	CB	CYS	B	418	49.513	71.413	36.319	1.00	39.12
	2308	SG	CYS	B	418	48.782	69.912	37.050	1.00	53.87
	2309	N	ALA	B	419	52.429	69.541	36.654	1.00	42.75
	2310	CA	ALA	B	419	53.102	68.362	36.118	1.00	45.21
	2311	CB	ALA	B	419	54.527	68.243	36.688	1.00	45.00
	2312	C	ALA	B	419	52.265	67.138	36.498	1.00	46.28
	2313	O	ALA	B	419	52.172	66.774	37.671	1.00	44.60
	2314	N	VAL	B	420	51.639	66.512	35.508	1.00	49.65
	2315	CA	VAL	B	420	50.811	65.348	35.778	1.00	54.91
	2316	CB	VAL	B	420	49.584	65.305	34.855	1.00	52.57
	2317	CG1	VAL	B	420	48.742	64.085	35.189	1.00	54.41
	2318	CG2	VAL	B	420	48.756	66.568	35.017	1.00	52.89
	2319	C	VAL	B	420	51.572	64.036	35.623	1.00	59.75
	2320	O	VAL	B	420	52.083	63.723	34.544	1.00	56.32
	2321	N	THR	B	421	51.640	63.275	36.713	1.00	65.72
	2322	CA	THR	B	421	52.322	61.985	36.717	1.00	72.95
	2323	CB	THR	B	421	53.303	61.867	37.903	1.00	73.73
	2324	OG1	THR	B	421	54.294	62.898	37.818	1.00	78.26
	2325	CG2	THR	B	421	53.995	60.518	37.883	1.00	74.84
	2326	C	THR	B	421	51.302	60.859	36.831	1.00	76.77
	2327	O	THR	B	421	50.937	60.459	37.936	1.00	76.76
	2328	N	ALA	B	422	50.843	60.352	35.690	1.00	81.68
	2329	CA	ALA	B	422	49.862	59.270	35.673	1.00	86.81
	2330	CB	ALA	B	422	49.134	59.242	34.332	1.00	86.67
	2331	C	ALA	B	422	50.540	57.930	35.922	1.00	90.55
	2332	O	ALA	B	422	51.724	57.757	35.623	1.00	91.00
	2333	N	PRO	B	423	49.793	56.959	36.475	1.00	93.77
	2334	CD	PRO	B	423	48.340	56.985	36.715	1.00	94.85
	2335	CA	PRO	B	423	50.343	55.630	36.759	1.00	95.83

	2336	CB	PRO	B	423	49.141	54.869	37.309	1.00	96.70
	2337	CG	PRO	B	423	47.981	55.526	36.613	1.00	97.10
	2338	C	PRO	B	423	50.926	54.988	35.504	1.00	97.16
	2339	O	PRO	B	423	52.128	54.750	35.426	1.00	97.34
	2340	N	ALA	B	424	50.076	54.707	34.522	1.00	98.50
	2341	CA	ALA	B	424	50.537	54.114	33.271	1.00	99.73
	2342	CB	ALA	B	424	49.348	53.605	32.474	1.00	99.11
	2343	C	ALA	B	424	51.282	55.188	32.475	1.00	100.69
	2344	O	ALA	B	424	51.875	56.097	33.054	1.00	101.64
	2345	N	LEU	B	425	51.245	55.079	31.150	1.00	100.65
	2346	CA	LEU	B	425	51.895	56.050	30.272	1.00	99.91
	2347	CB	LEU	B	425	51.228	57.418	30.429	1.00	100.27
	2348	CG	LEU	B	425	49.767	57.474	29.975	1.00	102.88
	2349	CD1	LEU	B	425	49.214	58.865	30.211	1.00	102.68
	2350	CD2	LEU	B	425	49.668	57.102	28.497	1.00	105.00
	2351	C	LEU	B	425	53.400	56.173	30.514	1.00	98.82
	2352	O	LEU	B	425	53.924	55.615	31.471	1.00	98.87
	2353	N	PRO	B	426	54.115	56.888	29.625	1.00	97.69
	2354	CD	PRO	B	426	53.661	57.182	28.251	1.00	98.02
	2355	CA	PRO	B	426	55.566	57.087	29.739	1.00	95.83
	2356	CB	PRO	B	426	56.030	56.927	28.303	1.00	96.48
	2357	CG	PRO	B	426	54.941	57.635	27.555	1.00	96.97
	2358	C	PRO	B	426	55.949	58.455	30.309	1.00	94.21
	2359	O	PRO	B	426	56.240	58.594	31.498	1.00	94.03
	2360	N	ARG	B	427	55.963	59.460	29.439	1.00	92.33
	2361	CA	ARG	B	427	56.303	60.822	29.831	1.00	90.72
	2362	CB	ARG	B	427	56.583	61.672	28.590	1.00	92.36
	2363	CG	ARG	B	427	57.784	61.251	27.758	1.00	96.36
	2364	CD	ARG	B	427	59.015	62.075	28.102	1.00	99.46
	2365	NE	ARG	B	427	59.822	62.353	26.916	1.00	101.30
	2366	CZ	ARG	B	427	59.397	63.060	25.872	1.00	102.28
	2367	NH1	ARG	B	427	58.170	63.563	25.864	1.00	102.89
	2368	NH2	ARG	B	427	60.200	63.266	24.836	1.00	102.96
	2369	C	ARG	B	427	55.142	61.448	30.595	1.00	88.67
	2370	O	ARG	B	427	53.986	61.308	30.198	1.00	88.90
	2371	N	ALA	B	428	55.447	62.138	31.687	1.00	85.79
	2372	CA	ALA	B	428	54.412	62.793	32.469	1.00	82.45
	2373	CB	ALA	B	428	54.985	63.290	33.789	1.00	82.49
	2374	C	ALA	B	428	53.893	63.963	31.644	1.00	79.74
	2375	O	ALA	B	428	54.645	64.568	30.879	1.00	79.87
	2376	N	LEU	B	429	52.606	64.270	31.785	1.00	76.91
	2377	CA	LEU	B	429	51.996	65.377	31.051	1.00	72.60
	2378	CB	LEU	B	429	50.475	65.195	30.974	1.00	73.30
	2379	CG	LEU	B	429	49.915	63.916	30.343	1.00	75.14
	2380	CD1	LEU	B	429	48.403	63.894	30.500	1.00	70.88
	2381	CD2	LEU	B	429	50.304	63.844	28.873	1.00	79.00
	2382	C	LEU	B	429	52.310	66.679	31.777	1.00	69.58
	2383	O	LEU	B	429	52.391	66.706	33.006	1.00	67.68
	2384	N	MET	B	430	52.484	67.755	31.015	1.00	66.58
	2385	CA	MET	B	430	52.785	69.057	31.596	1.00	63.72
	2386	CB	MET	B	430	54.260	69.397	31.396	1.00	66.69
	2387	CG	MET	B	430	55.205	68.363	31.975	1.00	76.81
	2388	SD	MET	B	430	56.932	68.836	31.755	1.00	89.36
	2389	CE	MET	B	430	57.129	68.610	29.990	1.00	87.45
	2390	C	MET	B	430	51.926	70.150	30.981	1.00	59.15
	2391	O	MET	B	430	51.778	70.229	29.760	1.00	59.09
	2392	N	ARG	B	431	51.355	70.993	31.833	1.00	55.24
	2393	CA	ARG	B	431	50.509	72.077	31.354	1.00	51.07
	2394	CB	ARG	B	431	49.036	71.737	31.584	1.00	51.17
	2395	CG	ARG	B	431	48.661	70.309	31.203	1.00	55.59
	2396	CD	ARG	B	431	47.441	70.280	30.295	1.00	67.55
	2397	NE	ARG	B	431	47.784	70.453	28.884	1.00	74.62

	2398	CZ	ARG	B	431	48.220	69.472	28.099	1.00	76.90
	2399	NH1	ARG	B	431	48.364	68.247	28.586	1.00	77.02
	2400	NH2	ARG	B	431	48.513	69.712	26.826	1.00	79.64
	2401	C	ARG	B	431	50.868	73.356	32.087	1.00	47.90
	2402	O	ARG	B	431	51.214	73.323	33.268	1.00	46.26
	2403	N	SER	B	432	50.788	74.480	31.385	1.00	45.54
	2404	CA	SER	B	432	51.105	75.768	31.988	1.00	45.94
	2405	CB	SER	B	432	52.484	76.244	31.516	1.00	47.12
	2406	OG	SER	B	432	52.560	76.269	30.106	1.00	50.92
	2407	C	SER	B	432	50.063	76.836	31.688	1.00	43.27
	2408	O	SER	B	432	49.328	76.738	30.709	1.00	42.70
	2409	N	THR	B	433	50.012	77.864	32.531	1.00	40.97
	2410	CA	THR	B	433	49.048	78.937	32.342	1.00	38.90
	2411	CB	THR	B	433	47.725	78.633	33.073	1.00	39.50
	2412	OG1	THR	B	433	46.792	79.689	32.820	1.00	38.91
	2413	CG2	THR	B	433	47.954	78.507	34.584	1.00	36.51
	2414	C	THR	B	433	49.583	80.271	32.838	1.00	39.62
	2415	O	THR	B	433	50.412	80.317	33.744	1.00	39.87
	2416	N	THR	B	434	49.105	81.351	32.224	1.00	39.10
	2417	CA	THR	B	434	49.499	82.711	32.569	1.00	39.67
	2418	CB	THR	B	434	50.788	83.120	31.818	1.00	43.40
	2419	OG1	THR	B	434	50.496	83.293	30.425	1.00	53.59
	2420	CG2	THR	B	434	51.830	82.041	31.929	1.00	52.29
	2421	C	THR	B	434	48.380	83.661	32.131	1.00	38.41
	2422	O	THR	B	434	47.490	83.275	31.374	1.00	38.84
	2423	N	ALA	B	435	48.421	84.899	32.594	1.00	37.73
	2424	CA	ALA	B	435	47.410	85.853	32.189	1.00	44.38
	2425	CB	ALA	B	435	47.632	87.174	32.887	1.00	40.72
	2426	C	ALA	B	435	47.567	86.023	30.679	1.00	47.78
	2427	O	ALA	B	435	48.681	85.989	30.163	1.00	46.98
	2428	N	THR	B	436	46.454	86.187	29.971	1.00	52.31
	2429	CA	THR	B	436	46.506	86.383	28.526	1.00	55.83
	2430	CB	THR	B	436	45.131	86.108	27.860	1.00	59.83
	2431	OG1	THR	B	436	44.784	84.727	28.028	1.00	62.64
	2432	CG2	THR	B	436	45.175	86.441	26.368	1.00	60.56
	2433	C	THR	B	436	46.893	87.834	28.260	1.00	56.91
	2434	O	THR	B	436	46.358	88.748	28.888	1.00	55.51
	2435	N	SER	B	437	47.841	88.043	27.352	1.00	58.87
	2436	CA	SER	B	437	48.256	89.398	27.005	1.00	61.80
	2437	CB	SER	B	437	49.746	89.445	26.626	1.00	63.69
	2438	OG	SER	B	437	50.029	88.616	25.511	1.00	67.24
	2439	C	SER	B	437	47.397	89.847	25.828	1.00	61.35
	2440	O	SER	B	437	46.489	89.123	25.410	1.00	61.92
	2441	N	GLY	B	438	47.670	91.033	25.297	1.00	60.43
	2442	CA	GLY	B	438	46.881	91.513	24.177	1.00	59.27
	2443	C	GLY	B	438	45.909	92.601	24.590	1.00	58.25
	2444	O	GLY	B	438	45.753	92.861	25.779	1.00	58.13
	2445	N	PRO	B	439	45.237	93.253	23.628	1.00	58.84
	2446	CD	PRO	B	439	45.385	93.045	22.177	1.00	60.09
	2447	CA	PRO	B	439	44.277	94.325	23.897	1.00	57.04
	2448	CB	PRO	B	439	43.768	94.692	22.503	1.00	57.59
	2449	CG	PRO	B	439	44.933	94.376	21.628	1.00	59.40
	2450	C	PRO	B	439	43.147	93.909	24.828	1.00	54.66
	2451	O	PRO	B	439	42.824	92.723	24.945	1.00	56.08
	2452	N	ARG	B	440	42.548	94.897	25.482	1.00	51.95
	2453	CA	ARG	B	440	41.451	94.658	26.405	1.00	49.50
	2454	CB	ARG	B	440	41.829	95.129	27.817	1.00	51.89
	2455	CG	ARG	B	440	43.200	94.679	28.309	1.00	59.84
	2456	CD	ARG	B	440	43.266	93.188	28.635	1.00	66.22
	2457	NE	ARG	B	440	44.657	92.755	28.787	1.00	74.61
	2458	CZ	ARG	B	440	45.045	91.553	29.204	1.00	76.10
	2459	NH1	ARG	B	440	44.156	90.633	29.527	1.00	77.20

	2460	NH2	ARG	B	440	46.338	91.272	29.295	1.00	84.96
	2461	C	ARG	B	440	40.249	95.455	25.910	1.00	46.80
	2462	O	ARG	B	440	40.406	96.542	25.354	1.00	46.09
	2463	N	ALA	B	441	39.053	94.904	26.099	1.00	42.67
	2464	CA	ALA	B	441	37.821	95.576	25.698	1.00	39.13
	2465	CB	ALA	B	441	37.458	95.216	24.263	1.00	32.25
	2466	C	ALA	B	441	36.712	95.148	26.646	1.00	39.00
	2467	O	ALA	B	441	36.555	93.961	26.925	1.00	38.16
	2468	N	ALA	B	442	35.949	96.118	27.136	1.00	37.20
	2469	CA	ALA	B	442	34.861	95.864	28.063	1.00	37.26
	2470	CB	ALA	B	442	34.312	97.187	28.574	1.00	37.47
	2471	C	ALA	B	442	33.718	95.032	27.483	1.00	39.85
	2472	O	ALA	B	442	33.510	94.988	26.275	1.00	41.57
	2473	N	PRO	B	443	32.960	94.354	28.357	1.00	39.83
	2474	CD	PRO	B	443	33.303	94.122	29.766	1.00	40.96
	2475	CA	PRO	B	443	31.825	93.520	27.969	1.00	38.29
	2476	CB	PRO	B	443	31.678	92.542	29.144	1.00	36.98
	2477	CG	PRO	B	443	32.925	92.693	29.932	1.00	36.14
	2478	C	PRO	B	443	30.563	94.380	27.828	1.00	40.19
	2479	O	PRO	B	443	30.406	95.396	28.512	1.00	40.51
	2480	N	ALA	B	444	29.673	93.964	26.937	1.00	39.07
	2481	CA	ALA	B	444	28.412	94.658	26.724	1.00	36.58
	2482	CB	ALA	B	444	28.228	94.995	25.240	1.00	40.22
	2483	C	ALA	B	444	27.373	93.638	27.181	1.00	34.33
	2484	O	ALA	B	444	27.358	92.491	26.702	1.00	30.65
	2485	N	VAL	B	445	26.519	94.057	28.109	1.00	28.37
	2486	CA	VAL	B	445	25.520	93.172	28.664	1.00	26.39
	2487	CB	VAL	B	445	25.652	93.152	30.198	1.00	26.69
	2488	CG1	VAL	B	445	24.620	92.205	30.790	1.00	23.97
	2489	CG2	VAL	B	445	27.076	92.747	30.586	1.00	22.56
	2490	C	VAL	B	445	24.068	93.497	28.291	1.00	27.26
	2491	O	VAL	B	445	23.646	94.644	28.367	1.00	24.12
	2492	N	TYR	B	446	23.319	92.473	27.893	1.00	23.45
	2493	CA	TYR	B	446	21.919	92.645	27.541	1.00	25.54
	2494	CB	TYR	B	446	21.722	92.732	26.015	1.00	24.97
	2495	CG	TYR	B	446	20.264	92.896	25.660	1.00	24.95
	2496	CD1	TYR	B	446	19.517	93.961	26.182	1.00	37.39
	2497	CE1	TYR	B	446	18.146	94.094	25.907	1.00	34.09
	2498	CD2	TYR	B	446	19.613	91.973	24.851	1.00	28.20
	2499	CE2	TYR	B	446	18.245	92.092	24.567	1.00	31.02
	2500	CZ	TYR	B	446	17.519	93.160	25.102	1.00	34.30
	2501	OH	TYR	B	446	16.174	93.294	24.846	1.00	35.42
	2502	C	TYR	B	446	21.130	91.465	28.088	1.00	23.87
	2503	O	TYR	B	446	21.321	90.325	27.663	1.00	28.38
	2504	N	ALA	B	447	20.254	91.742	29.042	1.00	26.40
	2505	CA	ALA	B	447	19.445	90.707	29.671	1.00	27.30
	2506	CB	ALA	B	447	19.535	90.834	31.195	1.00	24.55
	2507	C	ALA	B	447	18.002	90.840	29.202	1.00	30.87
	2508	O	ALA	B	447	17.515	91.945	28.979	1.00	32.42
	2509	N	PHE	B	448	17.310	89.720	29.045	1.00	31.33
	2510	CA	PHE	B	448	15.939	89.799	28.582	1.00	34.25
	2511	CB	PHE	B	448	15.938	89.984	27.060	1.00	40.48
	2512	CG	PHE	B	448	16.497	88.805	26.314	1.00	39.26
	2513	CD1	PHE	B	448	15.663	87.763	25.923	1.00	39.27
	2514	CD2	PHE	B	448	17.862	88.704	26.059	1.00	36.97
	2515	CE1	PHE	B	448	16.180	86.633	25.286	1.00	43.41
	2516	CE2	PHE	B	448	18.389	87.578	25.422	1.00	36.78
	2517	CZ	PHE	B	448	17.546	86.541	25.036	1.00	37.14
	2518	C	PHE	B	448	15.113	88.579	28.952	1.00	34.75
	2519	O	PHE	B	448	15.646	87.554	29.369	1.00	34.97
	2520	N	ALA	B	449	13.801	88.708	28.798	1.00	37.02
	2521	CA	ALA	B	449	12.877	87.623	29.079	1.00	38.65

	2522	CB	ALA	B	449	11.731	88.122	39.898	1.00	32.34
	2523	C	ALA	B	449	12.350	87.050	27.767	1.00	42.92
	2524	O	ALA	B	449	12.165	87.774	26.794	1.00	42.07
	2525	N	THR	B	450	12.111	85.743	27.759	1.00	47.71
	2526	CA	THR	B	450	11.586	85.048	26.597	1.00	52.16
	2527	CB	THR	B	450	12.040	83.577	26.599	1.00	53.90
	2528	OG1	THR	B	450	13.468	83.522	26.685	1.00	61.82
	2529	CG2	THR	B	450	11.594	82.877	25.327	1.00	62.58
	2530	C	THR	B	450	10.053	85.097	26.607	1.00	54.69
	2531	O	THR	B	450	9.421	84.983	27.659	1.00	51.28
	2532	N	PRO	B	451	9.439	85.280	25.431	1.00	57.24
	2533	CD	PRO	B	451	10.061	85.618	24.137	1.00	60.66
	2534	CA	PRO	B	451	7.977	85.339	25.338	1.00	61.04
	2535	CB	PRO	B	451	7.736	85.571	23.846	1.00	61.38
	2536	CG	PRO	B	451	8.946	86.360	23.433	1.00	63.63
	2537	C	PRO	B	451	7.301	84.063	25.847	1.00	63.11
	2538	O	PRO	B	451	7.682	82.949	25.484	1.00	61.66
	2539	N	GLU	B	452	6.303	84.230	26.706	1.00	66.04
	2540	CA	GLU	B	452	5.575	83.083	27.237	1.00	69.40
	2541	CB	GLU	B	452	5.800	82.954	28.753	1.00	67.34
	2542	CG	GLU	B	452	5.911	81.505	29.277	1.00	60.86
	2543	CD	GLU	B	452	7.225	80.815	28.876	1.00	59.08
	2544	OE1	GLU	B	452	8.255	81.510	28.775	1.00	62.62
	2545	OE2	GLU	B	452	7.249	79.578	28.676	1.00	45.82
	2546	C	GLU	B	452	4.090	83.278	26.930	1.00	71.98
	2547	O	GLU	B	452	3.360	83.895	27.705	1.00	70.35
	2548	N	ALA	B	453	3.659	82.758	25.783	1.00	75.33
	2549	CA	ALA	B	453	2.266	82.867	25.347	1.00	78.80
	2550	CB	ALA	B	453	2.075	82.118	24.029	1.00	80.74
	2551	C	ALA	B	453	1.282	82.340	26.394	1.00	80.53
	2552	O	ALA	B	453	1.599	81.433	27.167	1.00	82.95
	2553	N	LYS	B	459	8.685	75.798	30.647	1.00	51.87
	2554	CA	LYS	B	459	9.250	76.647	31.693	1.00	52.84
	2555	CB	LYS	B	459	10.479	75.987	32.317	1.00	55.20
	2556	CG	LYS	B	459	10.171	74.721	33.089	1.00	63.98
	2557	CD	LYS	B	459	11.271	74.401	34.088	1.00	72.67
	2558	CE	LYS	B	459	11.366	75.484	35.157	1.00	77.63
	2559	NZ	LYS	B	459	12.302	75.122	36.259	1.00	83.78
	2560	C	LYS	B	459	9.638	78.033	31.195	1.00	50.86
	2561	O	LYS	B	459	10.211	78.174	30.118	1.00	49.65
	2562	N	ARG	B	460	9.332	79.045	32.001	1.00	48.30
	2563	CA	ARG	B	460	9.640	80.433	31.674	1.00	47.61
	2564	CB	ARG	B	460	8.865	81.350	32.620	1.00	51.65
	2565	CG	ARG	B	460	7.371	81.029	32.591	1.00	59.85
	2566	CD	ARG	B	460	6.570	81.784	33.635	1.00	65.41
	2567	NE	ARG	B	460	5.158	81.400	33.603	1.00	70.36
	2568	CZ	ARG	B	460	4.702	80.174	33.848	1.00	73.06
	2569	NH1	ARG	B	460	5.540	79.188	34.150	1.00	75.61
	2570	NH2	ARG	B	460	3.401	79.929	33.791	1.00	76.52
	2571	C	ARG	B	460	11.154	80.664	31.759	1.00	44.39
	2572	O	ARG	B	460	11.839	80.058	32.589	1.00	41.11
	2573	N	THR	B	461	11.672	81.540	30.905	1.00	40.18
	2574	CA	THR	B	461	13.111	81.768	30.850	1.00	40.02
	2575	CB	THR	B	461	13.733	80.985	29.659	1.00	41.84
	2576	OG1	THR	B	461	13.383	79.601	29.750	1.00	52.98
	2577	CG2	THR	B	461	15.238	81.102	29.666	1.00	48.91
	2578	C	THR	B	461	13.574	83.207	30.699	1.00	37.19
	2579	O	THR	B	461	12.959	84.009	29.982	1.00	37.94
	2580	N	LEU	B	462	14.681	83.512	31.375	1.00	33.00
	2581	CA	LEU	B	462	15.335	84.809	31.289	1.00	29.46
	2582	CB	LEU	B	462	15.550	85.434	32.667	1.00	30.35

	2583	CG	LEU	B	462	14.282	85.678	33.498	1.00	33.09
	2584	CD1	LEU	B	462	14.639	86.412	34.785	1.00	32.32
	2585	CD2	LEU	B	462	13.293	86.499	32.699	1.00	25.52
	2586	C	LEU	B	462	16.672	84.439	30.662	1.00	29.44
	2587	O	LEU	B	462	17.184	83.339	30.894	1.00	24.62
	2588	N	ALA	B	463	17.237	85.343	29.868	1.00	27.23
	2589	CA	ALA	B	463	18.486	85.050	29.192	1.00	27.78
	2590	CB	ALA	B	463	18.199	84.488	27.790	1.00	26.61
	2591	C	ALA	B	463	19.332	86.301	29.104	1.00	28.37
	2592	O	ALA	B	463	18.824	87.415	29.233	1.00	29.09
	2593	N	CYS	B	464	20.623	86.115	28.870	1.00	22.40
	2594	CA	CYS	B	464	21.534	87.246	28.821	1.00	26.72
	2595	C	CYS	B	464	22.622	87.038	27.786	1.00	24.16
	2596	O	CYS	B	464	23.199	85.952	27.691	1.00	23.01
	2597	CB	CYS	B	464	22.172	87.410	30.200	1.00	24.58
	2598	SG	CYS	B	464	23.327	88.794	30.423	1.00	40.31
	2599	N	LEU	B	465	22.908	88.096	27.032	1.00	22.68
	2600	CA	LEU	B	465	23.950	88.052	26.013	1.00	24.31
	2601	CB	LEU	B	465	23.390	88.473	24.640	1.00	26.81
	2602	CG	LEU	B	465	24.419	88.841	23.554	1.00	21.10
	2603	CD1	LEU	B	465	25.310	87.659	23.251	1.00	21.73
	2604	CD2	LEU	B	465	23.700	89.262	22.293	1.00	30.90
	2605	C	LEU	B	465	25.043	89.013	26.453	1.00	23.79
	2606	O	LEU	B	465	24.770	90.183	26.741	1.00	22.87
	2607	N	ILE	B	466	26.276	88.521	26.510	1.00	23.16
	2608	CA	ILE	B	466	27.402	89.349	26.926	1.00	23.50
	2609	CB	ILE	B	466	28.018	88.838	28.251	1.00	23.66
	2610	CG2	ILE	B	466	29.140	89.800	28.705	1.00	29.47
	2611	CG1	ILE	B	466	26.913	88.739	29.320	1.00	19.89
	2612	CD1	ILE	B	466	27.398	88.229	30.650	1.00	36.91
	2613	C	ILE	B	466	28.388	89.274	25.784	1.00	22.24
	2614	O	ILE	B	466	28.811	88.189	25.385	1.00	24.74
	2615	N	GLN	B	467	28.789	90.433	25.270	1.00	23.91
	2616	CA	GLN	B	467	29.642	90.418	24.095	1.00	31.01
	2617	CB	GLN	B	467	28.747	90.376	22.846	1.00	30.11
	2618	CG	GLN	B	467	27.869	91.607	22.654	1.00	26.37
	2619	CD	GLN	B	467	26.920	91.486	21.464	1.00	29.83
	2620	OE1	GLN	B	467	27.136	90.710	20.521	1.00	28.59
	2621	NE2	GLN	B	467	25.869	92.282	21.495	1.00	31.49
	2622	C	GLN	B	467	30.641	91.546	23.952	1.00	33.72
	2623	O	GLN	B	467	30.691	92.469	24.768	1.00	31.53
	2624	N	ASN	B	468	31.442	91.421	22.895	1.00	38.27
	2625	CA	ASN	B	468	32.465	92.385	22.526	1.00	41.08
	2626	CB	ASN	B	468	31.839	93.744	22.245	1.00	43.70
	2627	CG	ASN	B	468	30.665	93.651	21.303	1.00	50.48
	2628	OD1	ASN	B	468	30.722	92.959	20.281	1.00	59.45
	2629	ND2	ASN	B	468	29.594	94.357	21.628	1.00	56.28
	2630	C	ASN	B	468	33.560	92.548	23.554	1.00	41.04
	2631	O	ASN	B	468	34.155	93.614	23.660	1.00	38.53
	2632	N	PHE	B	469	33.843	91.499	24.309	1.00	38.66
	2633	CA	PHE	B	469	34.894	91.604	25.303	1.00	38.07
	2634	CB	PHE	B	469	34.360	91.181	26.673	1.00	29.35
	2635	CG	PHE	B	469	34.064	89.712	26.791	1.00	28.48
	2636	CD1	PHE	B	469	35.059	88.815	27.113	1.00	23.56
	2637	CD2	PHE	B	469	32.777	89.231	26.579	1.00	24.16
	2638	CE1	PHE	B	469	34.784	87.463	27.228	1.00	27.41
	2639	CE2	PHE	B	469	32.493	87.867	26.691	1.00	32.69
	2640	CZ	PHE	B	469	33.506	86.984	27.017	1.00	24.40
	2641	C	PHE	B	469	36.125	90.785	24.939	1.00	38.11

	2642	O	PHE	B	469	36.026	89.752	24.287	1.00	39.11
	2643	N	MET	B	470	37.287	91.267	25.359	1.00	40.05
	2644	CA	MET	B	470	38.569	90.599	25.130	1.00	41.39
	2645	CB	MET	B	470	39.183	90.982	23.779	1.00	46.13
	2646	CG	MET	B	470	39.557	92.441	23.570	1.00	60.40
	2647	SD	MET	B	470	39.966	92.737	21.820	1.00	65.64
	2648	CE	MET	B	470	41.659	92.059	21.727	1.00	71.36
	2649	C	MET	B	470	39.417	91.095	26.280	1.00	38.04
	2650	O	MET	B	470	39.376	92.273	26.618	1.00	36.87
	2651	N	PRO	B	471	40.184	90.201	26.925	1.00	37.84
	2652	CD	PRO	B	471	40.913	90.654	28.117	1.00	38.40
	2653	CA	PRO	B	471	40.360	88.747	26.742	1.00	37.04
	2654	CB	PRO	B	471	41.485	88.400	27.732	1.00	38.82
	2655	CG	PRO	B	471	42.076	89.748	28.096	1.00	40.26
	2656	C	PRO	B	471	39.092	87.915	26.996	1.00	35.06
	2657	O	PRO	B	471	38.076	88.443	27.432	1.00	33.27
	2658	N	GLU	B	472	39.180	86.611	26.760	1.00	35.63
	2659	CA	GLU	B	472	38.033	85.705	26.898	1.00	38.83
	2660	CB	GLU	B	472	38.292	84.431	26.109	1.00	43.92
	2661	CG	GLU	B	472	39.299	83.516	26.792	1.00	54.98
	2662	CD	GLU	B	472	39.657	82.288	25.963	1.00	65.38
	2663	OE1	GLU	B	472	39.172	82.169	24.821	1.00	73.96
	2664	OE2	GLU	B	472	40.433	81.442	26.450	1.00	71.17
	2665	C	GLU	B	472	37.568	85.292	28.294	1.00	36.65
	2666	O	GLU	B	472	36.453	84.801	28.451	1.00	32.41
	2667	N	ASP	B	473	38.402	85.482	29.311	1.00	35.48
	2668	CA	ASP	B	473	38.004	85.092	30.668	1.00	34.00
	2669	CB	ASP	B	473	39.225	85.066	31.594	1.00	39.24
	2670	CG	ASP	B	473	40.239	83.993	31.193	1.00	48.86
	2671	OD1	ASP	B	473	39.800	82.876	30.817	1.00	42.86
	2672	OD2	ASP	B	473	41.461	84.270	31.265	1.00	46.87
	2673	C	ASP	B	473	36.917	85.993	31.256	1.00	34.33
	2674	O	ASP	B	473	37.057	87.220	31.315	1.00	34.18
	2675	N	ILE	B	474	35.824	85.384	31.691	1.00	27.93
	2676	CA	ILE	B	474	34.738	86.165	32.254	1.00	28.40
	2677	CB	ILE	B	474	33.848	86.726	31.129	1.00	25.16
	2678	CG2	ILE	B	474	33.036	85.602	30.489	1.00	26.53
	2679	CG1	ILE	B	474	32.935	87.828	31.664	1.00	21.56
	2680	CD1	ILE	B	474	32.219	88.591	30.507	1.00	23.93
	2681	C	ILE	B	474	33.890	85.326	33.190	1.00	26.83
	2682	O	ILE	B	474	33.773	84.127	33.014	1.00	25.94
	2683	N	SER	B	475	33.325	85.975	34.202	1.00	24.54
	2684	CA	SER	B	475	32.446	85.336	35.167	1.00	23.71
	2685	CB	SER	B	475	32.932	85.586	36.590	1.00	22.00
	2686	OG	SER	B	475	34.221	85.045	36.759	1.00	30.00
	2687	C	SER	B	475	31.071	85.967	34.983	1.00	24.55
	2688	O	SER	B	475	30.931	87.190	34.965	1.00	23.24
	2689	N	VAL	B	476	30.058	85.124	34.847	1.00	24.48
	2690	CA	VAL	B	476	28.692	85.562	34.654	1.00	26.25
	2691	CB	VAL	B	476	28.097	84.928	33.379	1.00	24.14
	2692	CG1	VAL	B	476	26.635	85.340	33.227	1.00	23.36
	2693	CG2	VAL	B	476	28.907	85.357	32.163	1.00	28.16
	2694	C	VAL	B	476	27.877	85.111	35.847	1.00	28.80
	2695	O	VAL	B	476	28.045	83.993	36.339	1.00	32.13
	2696	N	GLN	B	477	26.993	85.971	36.326	1.00	28.79
	2697	CA	GLN	B	477	26.176	85.589	37.458	1.00	30.02
	2698	CB	GLN	B	477	26.913	85.854	38.774	1.00	31.30
	2699	CG	GLN	B	477	27.360	87.270	38.993	1.00	46.28
	2700	CD	GLN	B	477	28.499	87.368	40.007	1.00	49.95
	2701	OE1	GLN	B	477	28.842	88.455	40.465	1.00	51.94
	2702	NE2	GLN	B	477	29.097	86.227	40.349	1.00	51.51
	2703	C	GLN	B	477	24.856	86.313	37.431	1.00	30.41

	2704	O	GLN	B	477	24.757	87.415	36.902	1.00	30.03
	2705	N	TRP	B	478	23.841	85.659	37.976	1.00	29.86
	2706	CA	TRP	B	478	22.505	86.210	38.042	1.00	29.12
	2707	CB	TRP	B	478	21.499	85.165	37.579	1.00	31.11
	2708	CG	TRP	B	478	21.527	84.936	36.112	1.00	36.98
	2709	CD2	TRP	B	478	20.726	85.605	35.132	1.00	34.77
	2710	CE2	TRP	B	478	21.092	85.084	33.870	1.00	37.75
	2711	CE3	TRP	B	478	19.742	86.602	35.194	1.00	31.61
	2712	CD1	TRP	B	478	22.320	84.060	35.432	1.00	35.86
	2713	NE1	TRP	B	478	22.065	84.142	34.086	1.00	35.58
	2714	CZ2	TRP	B	478	20.494	85.521	32.668	1.00	26.96
	2715	CZ3	TRP	B	478	19.148	87.039	34.005	1.00	35.86
	2716	CH2	TRP	B	478	19.531	86.497	32.757	1.00	31.66
	2717	C	TRP	B	478	22.175	86.648	39.468	1.00	29.01
	2718	O	TRP	B	478	22.580	86.006	40.439	1.00	24.19
	2719	N	LEU	B	479	21.436	87.742	39.582	1.00	31.15
	2720	CA	LEU	B	479	21.042	88.275	40.880	1.00	36.67
	2721	CB	LEU	B	479	21.837	89.537	41.198	1.00	41.07
	2722	CG	LEU	B	479	23.328	89.584	40.867	1.00	48.71
	2723	CD1	LEU	B	479	23.889	90.861	41.440	1.00	57.57
	2724	CD2	LEU	B	479	24.054	88.396	41.455	1.00	56.00
	2725	C	LEU	B	479	19.556	88.624	40.920	1.00	38.99
	2726	O	LEU	B	479	18.965	88.998	39.909	1.00	37.96
	2727	N	HIS	B	480	18.963	88.500	42.096	1.00	42.00
	2728	CA	HIS	B	480	17.561	88.834	42.284	1.00	48.67
	2729	CB	HIS	B	480	16.784	87.648	42.871	1.00	50.22
	2730	CG	HIS	B	480	15.309	87.894	43.014	1.00	53.99
	2731	CD2	HIS	B	480	14.256	87.041	42.993	1.00	56.80
	2732	ND1	HIS	B	480	14.779	89.147	43.239	1.00	54.56
	2733	CE1	HIS	B	480	13.465	89.057	43.348	1.00	60.76
	2734	NE2	HIS	B	480	13.122	87.789	43.203	1.00	59.92
	2735	C	HIS	B	480	17.625	89.972	43.283	1.00	52.66
	2736	O	HIS	B	480	17.426	89.777	44.482	1.00	51.85
	2737	N	ASN	B	481	17.945	91.161	42.780	1.00	58.88
	2738	CA	ASN	B	481	18.062	92.339	43.628	1.00	63.74
	2739	CB	ASN	B	481	16.763	92.588	44.407	1.00	69.70
	2740	CG	ASN	B	481	15.674	93.211	43.561	1.00	76.04
	2741	OD1	ASN	B	481	14.513	93.246	43.962	1.00	80.67
	2742	ND2	ASN	B	481	16.042	93.719	42.392	1.00	82.88
	2743	C	ASN	B	481	19.182	92.134	44.633	1.00	63.93
	2744	O	ASN	B	481	19.008	91.402	45.604	1.00	67.09
	2745	N	GLU	B	482	20.322	92.781	44.399	1.00	62.43
	2746	CA	GLU	B	482	21.477	92.715	45.299	1.00	60.15
	2747	CB	GLU	B	482	21.225	93.623	46.519	1.00	65.85
	2748	CG	GLU	B	482	19.754	94.021	46.707	1.00	78.14
	2749	CD	GLU	B	482	19.282	93.946	48.144	1.00	84.88
	2750	OE1	GLU	B	482	19.662	92.984	48.846	1.00	90.19
	2751	OE2	GLU	B	482	18.518	94.841	48.566	1.00	87.19
	2752	C	GLU	B	482	21.949	91.331	45.786	1.00	54.93
	2753	O	GLU	B	482	23.084	91.194	46.247	1.00	57.04
	2754	N	VAL	B	483	21.111	90.305	45.686	1.00	49.03
	2755	CA	VAL	B	483	21.511	88.987	46.163	1.00	45.46
	2756	CB	VAL	B	483	20.450	88.391	47.126	1.00	43.71
	2757	CG1	VAL	B	483	19.099	88.280	46.427	1.00	50.19
	2758	CG2	VAL	B	483	20.913	87.033	47.633	1.00	43.76
	2759	C	VAL	B	483	21.758	88.016	45.022	1.00	43.31
	2760	O	VAL	B	483	20.924	87.859	44.137	1.00	41.21
	2761	N	GLN	B	484	22.913	87.362	45.061	1.00	42.10
	2762	CA	GLN	B	484	23.303	86.411	44.036	1.00	41.31
	2763	CB	GLN	B	484	24.822	86.251	44.047	1.00	46.93
	2764	CG	GLN	B	484	25.338	85.180	43.107	1.00	54.66
	2765	CD	GLN	B	484	26.851	85.172	42.999	1.00	61.50

	2766	OE1	GLN	B	484	27.442	84.198	42.532	1.00	65.59
	2767	NE2	GLN	B	484	27.486	86.267	43.416	1.00	62.36
	2768	C	GLN	B	484	22.642	85.036	44.141	1.00	40.69
	2769	O	GLN	B	484	22.503	84.476	45.232	1.00	39.56
	2770	N	LEU	B	485	22.242	84.502	42.989	1.00	34.74
	2771	CA	LEU	B	485	21.602	83.192	42.909	1.00	36.73
	2772	CB	LEU	B	485	20.721	83.089	41.655	1.00	36.78
	2773	CG	LEU	B	485	19.589	84.099	41.457	1.00	38.16
	2774	CD1	LEU	B	485	18.876	83.831	40.134	1.00	39.22
	2775	CD2	LEU	B	485	18.631	83.993	42.621	1.00	41.68
	2776	C	LEU	B	485	22.677	82.115	42.834	1.00	36.82
	2777	O	LEU	B	485	23.805	82.388	42.440	1.00	34.53
	2778	N	PRO	B	486	22.342	80.875	43.217	1.00	40.02
	2779	CD	PRO	B	486	21.037	80.349	43.652	1.00	39.74
	2780	CA	PRO	B	486	23.351	79.809	43.151	1.00	45.08
	2781	CB	PRO	B	486	22.606	78.582	43.678	1.00	44.97
	2782	CG	PRO	B	486	21.438	79.143	44.439	1.00	41.94
	2783	C	PRO	B	486	23.738	79.629	41.687	1.00	49.91
	2784	O	PRO	B	486	22.889	79.770	40.809	1.00	49.23
	2785	N	ASP	B	487	25.001	79.309	41.423	1.00	54.02
	2786	CA	ASP	B	487	25.469	79.114	40.054	1.00	58.50
	2787	CB	ASP	B	487	26.953	78.749	40.061	1.00	68.77
	2788	CG	ASP	B	487	27.607	78.938	38.708	1.00	79.77
	2789	OD1	ASP	B	487	27.055	78.436	37.703	1.00	87.08
	2790	OD2	ASP	B	487	28.679	79.584	38.652	1.00	87.04
	2791	C	ASP	B	487	24.672	78.006	39.354	1.00	57.99
	2792	O	ASP	B	487	24.248	78.155	38.202	1.00	58.25
	2793	N	ALA	B	488	24.465	76.905	40.071	1.00	55.74
	2794	CA	ALA	B	488	23.739	75.748	39.554	1.00	55.27
	2795	CB	ALA	B	488	23.478	74.767	40.682	1.00	55.02
	2796	C	ALA	B	488	22.423	76.089	38.861	1.00	54.82
	2797	O	ALA	B	488	21.874	75.274	38.117	1.00	55.09
	2798	N	ARG	B	489	21.918	77.293	39.096	1.00	52.93
	2799	CA	ARG	B	489	20.656	77.701	38.501	1.00	48.90
	2800	CB	ARG	B	489	20.029	78.801	39.351	1.00	47.45
	2801	CG	ARG	B	489	19.257	78.264	40.537	1.00	49.40
	2802	CD	ARG	B	489	17.772	78.337	40.256	1.00	52.76
	2803	NE	ARG	B	489	17.174	79.497	40.910	1.00	60.57
	2804	CZ	ARG	B	489	16.041	80.087	40.540	1.00	60.40
	2805	NH1	ARG	B	489	15.353	79.641	39.496	1.00	61.65
	2806	NH2	ARG	B	489	15.587	81.120	41.234	1.00	62.45
	2807	C	ARG	B	489	20.706	78.144	37.042	1.00	45.96
	2808	O	ARG	B	489	19.688	78.099	36.354	1.00	45.86
	2809	N	HIS	B	490	21.867	78.568	36.559	1.00	41.69
	2810	CA	HIS	B	490	21.945	79.020	35.172	1.00	38.41
	2811	CB	HIS	B	490	22.314	80.513	35.103	1.00	39.34
	2812	CG	HIS	B	490	23.703	80.825	35.570	1.00	38.03
	2813	CD2	HIS	B	490	24.885	80.816	34.911	1.00	41.49
	2814	ND1	HIS	B	490	23.994	81.157	36.876	1.00	44.03
	2815	CE1	HIS	B	490	25.298	81.337	37.001	1.00	42.68
	2816	NE2	HIS	B	490	25.860	81.135	35.823	1.00	46.75
	2817	C	HIS	B	490	22.921	78.218	34.322	1.00	37.56
	2818	O	HIS	B	490	23.748	77.483	34.840	1.00	38.74
	2819	N	SER	B	491	22.804	78.359	33.006	1.00	36.46
	2820	CA	SER	B	491	23.694	77.674	32.079	1.00	35.63
	2821	CB	SER	B	491	22.902	76.660	31.255	1.00	34.76
	2822	OG	SER	B	491	23.751	75.950	30.374	1.00	51.24
	2823	C	SER	B	491	24.355	78.712	31.165	1.00	32.46
	2824	O	SER	B	491	23.672	79.478	30.482	1.00	34.26
	2825	N	THR	B	492	25.681	78.732	31.154	1.00	30.35
	2826	CA	THR	B	492	26.453	79.678	30.350	1.00	32.31
	2827	CB	THR	B	492	27.421	80.496	31.263	1.00	33.20

	2828	OG1	THR	B	492	26.667	81.141	32.294	1.00	38.93
	2829	CG2	THR	B	492	28.185	81.554	30.478	1.00	30.28
	2830	C	THR	B	492	27.272	78.961	29.265	1.00	32.83
	2831	O	THR	B	492	27.930	77.962	29.535	1.00	34.30
	2832	N	THR	B	493	27.240	79.482	28.042	1.00	32.82
	2833	CA	THR	B	493	27.990	78.881	26.939	1.00	32.09
	2834	CB	THR	B	493	27.449	79.346	25.570	1.00	27.96
	2835	OG1	THR	B	493	27.541	80.775	25.470	1.00	29.42
	2836	CG2	THR	B	493	26.000	78.920	25.406	1.00	21.13
	2837	C	THR	B	493	29.469	79.264	27.033	1.00	34.06
	2838	O	THR	B	493	29.830	80.164	27.783	1.00	31.49
	2839	N	GLN	B	494	30.318	78.570	26.284	1.00	35.84
	2840	CA	GLN	B	494	31.752	78.860	26.276	1.00	40.51
	2841	CB	GLN	B	494	32.544	77.671	25.718	1.00	46.41
	2842	CG	GLN	B	494	32.522	76.431	26.596	1.00	63.89
	2843	CD	GLN	B	494	33.008	76.710	28.007	1.00	72.04
	2844	OE1	GLN	B	494	34.053	77.328	28.206	1.00	77.06
	2845	NE2	GLN	B	494	32.250	76.245	28.996	1.00	81.58
	2846	C	GLN	B	494	32.004	80.088	25.409	1.00	39.51
	2847	O	GLN	B	494	31.330	80.296	24.402	1.00	38.74
	2848	N	PRO	B	495	32.977	80.924	25.795	1.00	38.63
	2849	CD	PRO	B	495	33.751	80.913	27.049	1.00	37.82
	2850	CA	PRO	B	495	33.270	82.120	25.000	1.00	39.10
	2851	CB	PRO	B	495	34.476	82.711	25.709	1.00	37.94
	2852	CG	PRO	B	495	34.212	82.345	27.146	1.00	43.34
	2853	C	PRO	B	495	33.569	81.746	23.551	1.00	41.43
	2854	O	PRO	B	495	34.254	80.762	23.292	1.00	42.40
	2855	N	ARG	B	496	33.033	82.514	22.613	1.00	41.33
	2856	CA	ARG	B	496	33.257	82.257	21.194	1.00	46.41
	2857	CB	ARG	B	496	31.965	81.792	20.526	1.00	44.11

	2858	CG	ARG	B	496	31.657	80.337	20.768	1.00	51.48
	2859	CD	ARG	B	496	30.269	79.967	20.287	1.00	56.73
	2860	NE	ARG	B	496	30.207	78.562	19.903	1.00	63.41
	2861	CZ	ARG	B	496	30.616	78.093	18.727	1.00	59.61
	2862	NH1	ARG	B	496	31.111	78.917	17.814	1.00	60.71
	2863	NH2	ARG	B	496	30.534	76.796	18.466	1.00	67.27
	2864	C	ARG	B	496	33.765	83.510	20.503	1.00	49.11
	2865	O	ARG	B	496	33.297	84.611	20.782	1.00	48.52
	2866	N	LYS	B	497	34.730	83.345	19.608	1.00	53.35
	2867	CA	LYS	B	497	35.278	84.484	18.892	1.00	60.05
	2868	CB	LYS	B	497	36.499	84.073	18.066	1.00	65.19
	2869	CG	LYS	B	497	37.713	83.690	18.888	1.00	75.27
	2870	CD	LYS	B	497	38.895	83.345	17.997	1.00	80.74
	2871	CE	LYS	B	497	40.130	83.066	18.831	1.00	86.89
	2872	NZ	LYS	B	497	41.322	82.746	17.997	1.00	91.84
	2873	C	LYS	B	497	34.224	85.054	17.969	1.00	62.05
	2874	O	LYS	B	497	33.209	84.416	17.697	1.00	61.50
	2875	N	THR	B	498	34.465	86.265	17.496	1.00	66.47
	2876	CA	THR	B	498	33.540	86.910	16.585	1.00	71.47
	2877	CB	THR	B	498	32.946	88.183	17.207	1.00	73.54
	2878	OG1	THR	B	498	33.619	88.482	18.434	1.00	77.08
	2879	CG2	THR	B	498	31.480	87.981	17.491	1.00	75.50
	2880	C	THR	B	498	34.281	87.261	15.306	1.00	72.65
	2881	O	THR	B	498	35.377	86.750	15.063	1.00	72.18
	2882	N	ALA	B	499	33.682	88.123	14.490	1.00	75.02
	2883	CA	ALA	B	499	34.297	88.538	13.233	1.00	77.01
	2884	CB	ALA	B	499	33.230	89.092	12.286	1.00	76.94
	2885	C	ALA	B	499	35.376	89.591	13.493	1.00	77.96
	2886	O	ALA	B	499	35.501	90.566	12.750	1.00	79.10
	2887	N	GLY	B	500	36.157	89.386	14.548	1.00	78.37
	2888	CA	GLY	B	500	37.210	90.327	14.883	1.00	78.64
	2889	C	GLY	B	500	36.855	91.208	16.068	1.00	77.71

	2890	O	GLY	B	500	37.722	91.859	16.653	1.00	78.53
	2891	N	SER	B	501	35.579	91.210	16.439	1.00	76.72
	2892	CA	SER	B	501	35.099	92.033	17.545	1.00	74.10
	2893	CB	SER	B	501	33.707	92.583	17.201	1.00	79.09
	2894	OG	SER	B	501	32.813	91.547	16.824	1.00	82.51
	2895	C	SER	B	501	35.055	91.365	18.924	1.00	70.47
	2896	O	SER	B	501	34.025	91.412	19.601	1.00	71.67
	2897	N	GLY	B	502	36.165	90.751	19.339	1.00	64.36
	2898	CA	GLY	B	502	36.231	90.116	20.653	1.00	55.25
	2899	C	GLY	B	502	35.489	88.801	20.889	1.00	48.43
	2900	O	GLY	B	502	35.445	87.931	20.019	1.00	47.45
	2901	N	PHE	B	503	34.922	88.648	22.085	1.00	41.96
	2902	CA	PHE	B	503	34.189	87.425	22.435	1.00	34.38
	2903	CB	PHE	B	503	34.925	86.625	23.518	1.00	34.97
	2904	CG	PHE	B	503	36.296	86.168	23.121	1.00	28.11
	2905	CD1	PHE	B	503	37.368	87.052	23.126	1.00	36.44
	2906	CD2	PHE	B	503	36.518	84.851	22.752	1.00	30.75
	2907	CE1	PHE	B	503	38.640	86.629	22.762	1.00	37.43
	2908	CE2	PHE	B	503	37.788	84.421	22.384	1.00	40.11
	2909	CZ	PHE	B	503	38.850	85.311	22.391	1.00	37.06
	2910	C	PHE	B	503	32.775	87.678	22.933	1.00	28.77
	2911	O	PHE	B	503	32.424	88.784	23.344	1.00	28.23
	2912	N	PHE	B	504	31.963	86.637	22.887	1.00	24.91
	2913	CA	PHE	B	504	30.594	86.713	23.357	1.00	25.79
	2914	CB	PHE	B	504	29.594	86.956	22.214	1.00	22.02
	2915	CG	PHE	B	504	29.343	85.766	21.326	1.00	30.92
	2916	CD1	PHE	B	504	28.300	84.878	21.601	1.00	32.77
	2917	CD2	PHE	B	504	30.113	85.563	20.181	1.00	34.76
	2918	CE1	PHE	B	504	28.030	83.804	20.751	1.00	29.72
	2919	CE2	PHE	B	504	29.852	84.493	19.326	1.00	33.59
	2920	CZ	PHE	B	504	28.801	83.613	19.620	1.00	34.51
	2921	C	PHE	B	504	30.272	85.425	24.073	1.00	28.90
	2922	O	PHE	B	504	30.849	84.378	23.783	1.00	26.02
	2923	N	VAL	B	505	29.348	85.529	25.020	1.00	25.50
	2924	CA	VAL	B	505	28.919	84.404	25.804	1.00	25.53
	2925	CB	VAL	B	505	29.709	84.407	27.145	1.00	29.70
	2926	CG1	VAL	B	505	29.124	85.416	28.098	1.00	25.34
	2927	CG2	VAL	B	505	29.763	83.037	27.735	1.00	35.22
	2928	C	VAL	B	505	27.404	84.585	26.008	1.00	26.24
	2929	O	VAL	B	505	26.893	85.705	26.004	1.00	22.25
	2930	N	PHE	B	506	26.687	83.475	26.150	1.00	28.62
	2931	CA	PHE	B	506	25.239	83.507	26.346	1.00	25.84
	2932	CB	PHE	B	506	24.539	82.831	25.165	1.00	29.19
	2933	CG	PHE	B	506	23.053	82.811	25.273	1.00	35.82
	2934	CD1	PHE	B	506	22.314	83.970	25.070	1.00	42.42
	2935	CD2	PHE	B	506	22.387	81.639	25.600	1.00	42.16
	2936	CE1	PHE	B	506	20.929	83.956	25.190	1.00	44.85
	2937	CE2	PHE	B	506	21.009	81.618	25.724	1.00	41.56
	2938	CZ	PHE	B	506	20.278	82.775	25.520	1.00	45.90
	2939	C	PHE	B	506	24.881	82.756	27.627	1.00	23.92
	2940	O	PHE	B	506	25.405	81.676	27.875	1.00	27.54
	2941	N	SER	B	507	23.982	83.314	28.423	1.00	25.96
	2942	CA	SER	B	507	23.559	82.675	29.668	1.00	25.75
	2943	CB	SER	B	507	24.119	83.456	30.865	1.00	24.23
	2944	OG	SER	B	507	23.643	82.926	32.088	1.00	33.35
	2945	C	SER	B	507	22.026	82.573	29.736	1.00	25.49
	2946	O	SER	B	507	21.316	83.530	29.452	1.00	25.61
	2947	N	ARG	B	508	21.537	81.397	30.106	1.00	26.99
	2948	CA	ARG	B	508	20.103	81.125	30.193	1.00	25.78
	2949	CB	ARG	B	508	19.779	79.948	29.275	1.00	24.46
	2950	CG	ARG	B	508	18.355	79.423	29.347	1.00	28.19
	2951	CD	ARG	B	508	18.251	78.191	28.462	1.00	27.68

	2952	NE	ARG	B	508	16.877	77.735	28.296	1.00	38.82
	2953	CZ	ARG	B	508	16.245	76.959	29.167	1.00	40.66
	2954	NH1	ARG	B	508	16.874	76.554	30.260	1.00	39.61
	2955	NH2	ARG	B	508	14.987	76.593	28.949	1.00	40.23
	2956	C	ARG	B	508	19.690	80.784	31.629	1.00	24.52
	2957	O	ARG	B	508	20.366	80.006	32.290	1.00	24.88
	2958	N	LEU	B	509	18.587	81.354	32.108	1.00	26.27
	2959	CA	LEU	B	509	18.110	81.088	33.478	1.00	31.33
	2960	CB	LEU	B	509	18.394	82.297	34.379	1.00	32.56
	2961	CG	LEU	B	509	17.826	82.289	35.808	1.00	33.39
	2962	CD1	LEU	B	509	18.551	81.250	36.666	1.00	27.13
	2963	CD2	LEU	B	509	17.986	83.679	36.409	1.00	27.35
	2964	C	LEU	B	509	16.612	80.770	33.550	1.00	33.20
	2965	O	LEU	B	509	15.777	81.654	33.379	1.00	35.36
	2966	N	GLU	B	510	16.270	79.509	33.814	1.00	33.43
	2967	CA	GLU	B	510	14.865	79.121	33.918	1.00	37.45
	2968	CB	GLU	B	510	14.720	77.598	33.795	1.00	38.70
	2969	CG	GLU	B	510	15.248	77.052	32.471	1.00	53.61
	2970	CD	GLU	B	510	14.878	75.591	32.203	1.00	62.03
	2971	OE1	GLU	B	510	15.161	74.723	33.058	1.00	65.31
	2972	OE2	GLU	B	510	14.310	75.312	31.124	1.00	63.62
	2973	C	GLU	B	510	14.315	79.593	35.259	1.00	37.95
	2974	O	GLU	B	510	14.965	79.413	36.292	1.00	35.84
	2975	N	VAL	B	511	13.134	80.209	35.255	1.00	37.36
	2976	CA	VAL	B	511	12.552	80.697	36.504	1.00	39.69
	2977	CB	VAL	B	511	12.588	82.234	36.587	1.00	29.12
	2978	CG1	VAL	B	511	14.010	82.725	36.411	1.00	28.52
	2979	CG2	VAL	B	511	11.667	82.836	35.546	1.00	31.67
	2980	C	VAL	B	511	11.110	80.243	36.708	1.00	45.51
	2981	O	VAL	B	511	10.444	79.824	35.756	1.00	46.84
	2982	N	THR	B	512	10.636	80.331	37.950	1.00	47.32
	2983	CA	THR	B	512	9.274	79.927	38.287	1.00	51.20
	2984	CB	THR	B	512	9.129	79.678	39.796	1.00	49.91
	2985	OG1	THR	B	512	9.458	80.877	40.508	1.00	46.57
	2986	CG2	THR	B	512	10.056	78.554	40.242	1.00	49.02
	2987	C	THR	B	512	8.288	81.015	37.887	1.00	54.77
	2988	O	THR	B	512	8.691	82.133	37.580	1.00	54.38
	2989	N	ARG	B	513	6.998	80.684	37.894	1.00	56.48
	2990	CA	ARG	B	513	5.958	81.645	37.535	1.00	56.58
	2991	CB	ARG	B	513	4.574	80.991	37.597	1.00	61.58
	2992	CG	ARG	B	513	3.570	81.570	36.611	1.00	67.62
	2993	CD	ARG	B	513	3.294	83.034	36.879	1.00	75.58
	2994	NE	ARG	B	513	2.863	83.743	35.678	1.00	83.06
	2995	CZ	ARG	B	513	2.519	85.028	35.652	1.00	86.37
	2996	NH1	ARG	B	513	2.551	85.744	36.764	1.00	88.41
	2997	NH2	ARG	B	513	2.154	85.602	34.515	1.00	87.87
	2998	C	ARG	B	513	5.997	82.817	38.500	1.00	55.15
	2999	O	ARG	B	513	5.744	83.961	38.117	1.00	55.55
	3000	N	ALA	B	514	6.319	82.524	39.755	1.00	55.02
	3001	CA	ALA	B	514	6.386	83.545	40.792	1.00	53.96
	3002	CB	ALA	B	514	6.628	82.885	42.139	1.00	53.56
	3003	C	ALA	B	514	7.472	84.585	40.505	1.00	54.12
	3004	O	ALA	B	514	7.187	85.781	40.419	1.00	54.41
	3005	N	GLU	B	515	8.716	84.136	40.364	1.00	54.63
	3006	CA	GLU	B	515	9.802	85.065	40.089	1.00	54.64
	3007	CB	GLU	B	515	11.166	84.375	40.238	1.00	58.15
	3008	CG	GLU	B	515	11.208	82.932	39.769	1.00	64.48
	3009	CD	GLU	B	515	12.493	82.221	40.174	1.00	65.38
	3010	OE1	GLU	B	515	12.957	82.417	41.316	1.00	66.84
	3011	OE2	GLU	B	515	13.037	81.451	39.359	1.00	68.35
	3012	C	GLU	B	515	9.644	85.671	38.705	1.00	54.36
	3013	O	GLU	B	515	10.240	86.703	38.406	1.00	51.06

	3014	N	TRP	B	516	8.831	85.037	37.863	1.00	55.85
	3015	CA	TRP	B	516	8.585	85.557	36.524	1.00	57.10
	3016	CB	TRP	B	516	7.845	84.538	35.653	1.00	58.50
	3017	CG	TRP	B	516	7.950	84.874	34.194	1.00	67.12
	3018	CD2	TRP	B	516	6.940	85.472	33.374	1.00	68.04
	3019	CE2	TRP	B	516	7.509	85.685	32.101	1.00	71.07
	3020	CE3	TRP	B	516	5.608	85.849	33.593	1.00	74.06
	3021	CD1	TRP	B	516	9.059	84.749	33.403	1.00	67.58
	3022	NE1	TRP	B	516	8.803	85.236	32.146	1.00	68.75
	3023	CZ2	TRP	B	516	6.793	86.263	31.048	1.00	75.59
	3024	CZ3	TRP	B	516	4.895	86.425	32.542	1.00	76.50
	3025	CH2	TRP	B	516	5.491	86.625	31.287	1.00	76.13
	3026	C	TRP	B	516	7.746	86.828	36.648	1.00	57.68
	3027	O	TRP	B	516	7.775	87.691	35.773	1.00	57.71
	3028	N	GLU	B	517	6.996	86.935	37.743	1.00	58.53
	3029	CA	GLU	B	517	6.173	88.113	38.008	1.00	60.83
	3030	CB	GLU	B	517	5.219	87.842	39.179	1.00	65.68
	3031	CG	GLU	B	517	3.832	87.363	38.775	1.00	77.69
	3032	CD	GLU	B	517	3.078	88.387	37.932	1.00	86.61
	3033	OE1	GLU	B	517	3.564	89.534	37.799	1.00	92.24
	3034	OE2	GLU	B	517	1.995	88.050	37.404	1.00	89.43
	3035	C	GLU	B	517	7.053	89.323	38.345	1.00	58.89
	3036	O	GLU	B	517	6.729	90.465	38.012	1.00	56.98
	3037	N	ALA	B	518	8.170	89.063	39.016	1.00	58.33
	3038	CA	ALA	B	518	9.097	90.121	39.398	1.00	54.78
	3039	CB	ALA	B	518	9.422	90.005	40.880	1.00	55.11
	3040	C	ALA	B	518	10.373	90.003	38.560	1.00	53.56
	3041	O	ALA	B	518	11.480	90.225	39.055	1.00	52.54
	3042	N	LYS	B	519	10.219	89.681	37.281	1.00	51.73
	3043	CA	LYS	B	519	11.383	89.508	36.429	1.00	52.62
	3044	CB	LYS	B	519	10.983	88.881	35.096	1.00	52.68
	3045	CG	LYS	B	519	10.253	89.792	34.146	1.00	53.71
	3046	CD	LYS	B	519	9.696	88.969	32.997	1.00	61.43
	3047	CE	LYS	B	519	8.899	89.819	32.036	1.00	65.64
	3048	NZ	LYS	B	519	8.140	88.958	31.098	1.00	74.93
	3049	C	LYS	B	519	12.160	90.786	36.185	1.00	52.55
	3050	O	LYS	B	519	13.313	90.743	35.761	1.00	49.84
	3051	N	ASP	B	520	11.533	91.920	36.462	1.00	54.27
	3052	CA	ASP	B	520	12.176	93.219	36.280	1.00	55.54
	3053	CB	ASP	B	520	11.146	94.337	36.431	1.00	65.40
	3054	CG	ASP	B	520	9.722	93.857	36.196	1.00	75.80
	3055	OD1	ASP	B	520	9.426	93.383	35.076	1.00	83.22
	3056	OD2	ASP	B	520	8.900	93.948	37.136	1.00	77.87
	3057	C	ASP	B	520	13.255	93.388	37.346	1.00	53.46
	3058	O	ASP	B	520	14.100	94.281	37.257	1.00	51.37
	3059	N	GLU	B	521	13.217	92.521	38.353	1.00	50.72
	3060	CA	GLU	B	521	14.178	92.584	39.442	1.00	50.66
	3061	CB	GLU	B	521	13.507	92.173	40.758	1.00	54.68
	3062	CG	GLU	B	521	12.510	93.192	41.301	1.00	61.75
	3063	CD	GLU	B	521	11.663	92.639	42.430	1.00	68.36
	3064	OE1	GLU	B	521	12.232	92.137	43.422	1.00	70.14
	3065	OE2	GLU	B	521	10.419	92.708	42.327	1.00	75.93
	3066	C	GLU	B	521	15.418	91.731	39.215	1.00	46.52
	3067	O	GLU	B	521	16.392	91.857	39.952	1.00	47.21
	3068	N	PHE	B	522	15.386	90.866	38.207	1.00	42.97
	3069	CA	PHE	B	522	16.531	90.011	37.919	1.00	38.46
	3070	CB	PHE	B	522	16.091	88.752	37.185	1.00	37.28
	3071	CG	PHE	B	522	15.420	87.754	38.076	1.00	42.52
	3072	CD1	PHE	B	522	14.090	87.925	38.454	1.00	44.12
	3073	CD2	PHE	B	522	16.133	86.671	38.592	1.00	40.14
	3074	CE1	PHE	B	522	13.474	87.036	39.338	1.00	48.02
	3075	CE2	PHE	B	522	15.528	85.775	39.477	1.00	42.77

	3076	CZ	PHE	B	522	14.192	85.960	39.852	1.00	41.32
	3077	C	PHE	B	522	17.594	90.748	37.130	1.00	36.02
	3078	O	PHE	B	522	17.292	91.474	36.182	1.00	37.87
	3079	N	ILE	B	523	18.842	90.558	37.539	1.00	32.13
	3080	CA	ILE	B	523	19.974	91.224	36.913	1.00	31.74
	3081	CB	ILE	B	523	20.634	92.208	37.908	1.00	36.58
	3082	CG2	ILE	B	523	21.849	92.889	37.262	1.00	38.36
	3083	CG1	ILE	B	523	19.600	93.233	38.386	1.00	39.38
	3084	CD1	ILE	B	523	20.086	94.083	39.536	1.00	40.35
	3085	C	ILE	B	523	21.041	90.244	36.430	1.00	30.51
	3086	O	ILE	B	523	21.306	89.231	37.066	1.00	29.34
	3087	N	CYS	B	524	21.651	90.554	35.298	1.00	28.73
	3088	CA	CYS	B	524	22.702	89.721	34.749	1.00	27.60
	3089	C	CYS	B	524	23.965	90.519	34.964	1.00	27.54
	3090	O	CYS	B	524	24.033	91.667	34.545	1.00	28.72
	3091	CB	CYS	B	524	22.477	89.504	33.251	1.00	26.75
	3092	SG	CYS	B	524	23.823	88.601	32.411	1.00	36.31
	3093	N	ARG	B	525	24.964	89.925	35.603	1.00	28.42
	3094	CA	ARG	B	525	26.200	90.634	35.874	1.00	28.35
	3095	CB	ARG	B	525	26.371	90.820	37.380	1.00	34.16
	3096	CG	ARG	B	525	27.688	91.480	37.769	1.00	39.75
	3097	CD	ARG	B	525	27.604	92.092	39.163	1.00	48.43
	3098	NE	ARG	B	525	27.775	91.117	40.226	1.00	52.97
	3099	CZ	ARG	B	525	27.492	91.358	41.502	1.00	58.72
	3100	NH1	ARG	B	525	27.020	92.546	41.867	1.00	55.56
	3101	NH2	ARG	B	525	27.670	90.410	42.414	1.00	55.90
	3102	C	ARG	B	525	27.416	89.927	35.317	1.00	28.14
	3103	O	ARG	B	525	27.545	88.711	35.409	1.00	28.95
	3104	N	ALA	B	526	28.317	90.708	34.743	1.00	25.82
	3105	CA	ALA	B	526	29.518	90.160	34.170	1.00	25.90
	3106	CB	ALA	B	526	29.614	90.544	32.691	1.00	28.82
	3107	C	ALA	B	526	30.697	90.729	34.931	1.00	27.38
	3108	O	ALA	B	526	30.701	91.910	35.253	1.00	24.32
	3109	N	VAL	B	527	31.676	89.882	35.245	1.00	24.37
	3110	CA	VAL	B	527	32.873	90.334	35.923	1.00	24.12
	3111	CB	VAL	B	527	33.166	89.546	37.201	1.00	24.30
	3112	CG1	VAL	B	527	34.510	89.963	37.762	1.00	26.10
	3113	CG2	VAL	B	527	32.083	89.804	38.224	1.00	30.97
	3114	C	VAL	B	527	33.954	90.077	34.902	1.00	26.78
	3115	O	VAL	B	527	34.078	88.969	34.375	1.00	25.10
	3116	N	HIS	B	528	34.743	91.103	34.630	1.00	26.18
	3117	CA	HIS	B	528	35.771	91.015	33.616	1.00	29.17
	3118	CB	HIS	B	528	35.110	91.187	32.221	1.00	28.69
	3119	CG	HIS	B	528	36.078	91.191	31.072	1.00	30.83
	3120	CD2	HIS	B	528	36.939	92.144	30.639	1.00	30.29
	3121	ND1	HIS	B	528	36.282	90.096	30.258	1.00	30.55
	3122	CE1	HIS	B	528	37.233	90.372	29.381	1.00	28.76
	3123	NE2	HIS	B	528	37.650	91.608	29.593	1.00	23.82
	3124	C	HIS	B	528	36.818	92.102	33.870	1.00	31.62
	3125	O	HIS	B	528	36.504	93.213	34.312	1.00	30.62
	3126	N	GLU	B	529	38.061	91.766	33.557	1.00	34.89
	3127	CA	GLU	B	529	39.200	92.651	33.753	1.00	41.27
	3128	CB	GLU	B	529	40.471	91.960	33.257	1.00	46.90
	3129	CG	GLU	B	529	41.692	92.879	33.228	1.00	61.52
	3130	CD	GLU	B	529	42.764	92.416	32.248	1.00	68.52
	3131	OE1	GLU	B	529	43.740	93.167	32.036	1.00	68.05
	3132	OE2	GLU	B	529	42.631	91.306	31.687	1.00	73.22
	3133	C	GLU	B	529	39.124	94.035	33.104	1.00	42.79

	3134	O	GLU	B	529	39.531	95.022	33.719	1.00	42.08
	3135	N	ALA	B	530	38.622	94.098	31.868	1.00	43.28
	3136	CA	ALA	B	530	38.539	95.350	31.113	1.00	44.89
	3137	CB	ALA	B	530	38.417	95.054	29.628	1.00	42.67
	3138	C	ALA	B	530	37.458	96.337	31.518	1.00	47.12
	3139	O	ALA	B	530	37.463	97.474	31.052	1.00	47.05
	3140	N	ALA	B	531	36.529	95.916	32.368	1.00	50.02
	3141	CA	ALA	B	531	35.470	96.808	32.820	1.00	54.71
	3142	CB	ALA	B	531	34.367	95.998	33.479	1.00	52.38
	3143	C	ALA	B	531	36.081	97.813	33.808	1.00	59.71
	3144	O	ALA	B	531	35.765	97.816	34.998	1.00	57.91
	3145	N	SER	B	532	36.958	98.664	33.275	1.00	66.39
	3146	CA	SER	B	532	37.701	99.689	34.022	1.00	71.61
	3147	CB	SER	B	532	37.651	101.030	33.272	1.00	75.15
	3148	OG	SER	B	532	36.326	101.410	32.932	1.00	81.74
	3149	C	SER	B	532	37.402	99.919	35.505	1.00	73.08
	3150	O	SER	B	532	38.293	99.745	36.343	1.00	75.98
	3151	N	PRO	B	533	36.167	100.321	35.864	1.00	72.21
	3152	CD	PRO	B	533	35.011	100.831	35.102	1.00	72.93
	3153	CA	PRO	B	533	35.956	100.524	37.299	1.00	69.88
	3154	CB	PRO	B	533	34.983	101.687	37.325	1.00	69.60
	3155	CG	PRO	B	533	34.063	101.322	36.205	1.00	71.96
	3156	C	PRO	B	533	35.388	99.283	37.987	1.00	67.12
	3157	O	PRO	B	533	34.331	98.780	37.600	1.00	67.77
	3158	N	SER	B	534	36.101	98.798	38.997	1.00	62.96
	3159	CA	SER	B	534	35.683	97.633	39.769	1.00	56.20
	3160	CB	SER	B	534	34.463	97.991	40.621	1.00	57.74
	3161	OG	SER	B	534	33.463	98.615	39.838	1.00	67.85
	3162	C	SER	B	534	35.406	96.342	38.989	1.00	49.03
	3163	O	SER	B	534	34.789	95.424	39.524	1.00	47.21
	3164	N	GLN	B	535	35.858	96.278	37.737	1.00	42.33
	3165	CA	GLN	B	535	35.704	95.096	36.896	1.00	38.93
	3166	CB	GLN	B	535	36.713	94.012	37.316	1.00	32.30
	3167	CG	GLN	B	535	38.181	94.388	37.128	1.00	35.25
	3168	CD	GLN	B	535	38.619	95.526	38.024	1.00	41.01
	3169	OE1	GLN	B	535	38.428	95.488	39.239	1.00	43.29
	3170	NE2	GLN	B	535	39.220	96.545	37.431	1.00	47.79
	3171	C	GLN	B	535	34.310	94.485	36.891	1.00	37.85
	3172	O	GLN	B	535	34.168	93.265	36.819	1.00	36.76
	3173	N	THR	B	536	33.283	95.320	36.953	1.00	37.28
	3174	CA	THR	B	536	31.925	94.805	36.955	1.00	39.00
	3175	CB	THR	B	536	31.319	94.848	38.366	1.00	41.53
	3176	OG1	THR	B	536	32.267	94.344	39.314	1.00	46.75
	3177	CG2	THR	B	536	30.076	93.987	38.424	1.00	39.44
	3178	C	THR	B	536	31.016	95.586	36.028	1.00	38.42
	3179	O	THR	B	536	31.148	96.794	35.895	1.00	43.26
	3180	N	VAL	B	537	30.105	94.877	35.374	1.00	37.42
	3181	CA	VAL	B	537	29.131	95.462	34.468	1.00	32.52
	3182	CB	VAL	B	537	29.619	95.466	32.990	1.00	36.29
	3183	CG1	VAL	B	537	28.580	96.148	32.114	1.00	35.71
	3184	CG2	VAL	B	537	30.931	96.205	32.859	1.00	43.42
	3185	C	VAL	B	537	27.876	94.594	34.562	1.00	31.41
	3186	O	VAL	B	537	27.946	93.369	34.435	1.00	31.67
	3187	N	GLN	B	538	26.726	95.219	34.787	1.00	27.91
	3188	CA	GLN	B	538	25.496	94.452	34.917	1.00	29.41
	3189	CB	GLN	B	538	25.231	94.136	36.392	1.00	29.17
	3190	CG	GLN	B	538	24.965	95.363	37.251	1.00	29.81
	3191	CD	GLN	B	538	24.710	94.983	38.691	1.00	29.58
	3192	OE1	GLN	B	538	25.443	94.176	39.267	1.00	37.40
	3193	NE2	GLN	B	538	23.676	95.559	39.285	1.00	32.13
	3194	C	GLN	B	538	24.304	95.193	34.356	1.00	31.40
	3195	O	GLN	B	538	24.314	96.411	34.256	1.00	33.62

	3196	N	ARG	B	539	23.267	94.449	34.002	1.00	31.64
	3197	CA	ARG	B	539	22.066	95.063	33.481	1.00	34.86
	3198	CB	ARG	B	539	22.120	95.120	31.955	1.00	41.64
	3199	CG	ARG	B	539	21.123	96.078	31.338	1.00	48.95
	3200	CD	ARG	B	539	21.796	96.845	30.216	1.00	59.63
	3201	NE	ARG	B	539	23.067	97.395	30.680	1.00	74.02
	3202	CZ	ARG	B	539	23.909	98.094	29.927	1.00	82.05
	3203	NH1	ARG	B	539	23.623	98.341	28.653	1.00	87.03
	3204	NH2	ARG	B	539	25.040	98.547	30.454	1.00	85.40
	3205	C	ARG	B	539	20.840	94.289	33.922	1.00	34.74
	3206	O	ARG	B	539	20.833	93.059	33.910	1.00	37.29
	3207	N	ALA	B	540	19.806	95.020	34.328	1.00	34.85
	3208	CA	ALA	B	540	18.561	94.408	34.756	1.00	34.24
	3209	CB	ALA	B	540	17.709	95.425	35.472	1.00	35.02
	3210	C	ALA	B	540	17.846	93.900	33.513	1.00	35.51
	3211	O	ALA	B	540	18.082	94.395	32.405	1.00	30.77
	3212	N	VAL	B	541	16.996	92.896	33.692	1.00	36.19
	3213	CA	VAL	B	541	16.251	92.326	32.580	1.00	42.85
	3214	CB	VAL	B	541	15.335	91.172	33.062	1.00	43.71
	3215	CG1	VAL	B	541	14.284	90.856	32.016	1.00	48.75
	3216	CG2	VAL	B	541	16.167	89.935	33.351	1.00	43.59
	3217	C	VAL	B	541	15.406	93.419	31.922	1.00	48.00
	3218	O	VAL	B	541	14.537	94.013	32.564	1.00	44.96
	3219	N	SER	B	542	15.673	93.694	30.649	1.00	53.41
	3220	CA	SER	B	542	14.914	94.717	29.948	1.00	61.94
	3221	CB	SER	B	542	15.564	95.068	28.606	1.00	62.96
	3222	OG	SER	B	542	15.462	94.004	27.679	1.00	69.91
	3223	C	SER	B	542	13.517	94.163	29.728	1.00	65.98
	3224	O	SER	B	542	13.347	92.972	29.466	1.00	67.12
	3225	N	VAL	B	543	12.520	95.029	29.851	1.00	70.21
	3226	CA	VAL	B	543	11.134	94.625	29.679	1.00	74.63
	3227	CB	VAL	B	543	10.479	94.300	31.042	1.00	78.23
	3228	CG1	VAL	B	543	9.026	93.887	30.840	1.00	79.65
	3229	CG2	VAL	B	543	11.256	93.191	31.741	1.00	79.80
	3230	C	VAL	B	543	10.341	95.729	28.989	1.00	75.67
	3231	O	VAL	B	543	9.847	96.626	29.704	1.00	77.58
	3232	OXT	VAL	B	543	10.240	95.693	27.744	1.00	74.95
	3233	C1	NAG	B	2	34.354	65.734	31.802	1.00	97.60
	3234	O1	NAG	B	2	33.245	65.687	30.975	1.00	99.81
	3235	C2	NAG	B	2	34.505	67.148	32.413	1.00	96.75
	3236	N2	NAG	B	2	33.295	67.525	33.111	1.00	98.55
	3237	C7	NAG	B	2	33.264	67.560	34.440	1.00	101.24
	3238	O7	NAG	B	2	34.215	67.219	35.144	1.00	100.19
	3239	C8	NAG	B	2	31.977	68.033	35.094	1.00	100.76
	3240	C3	NAG	B	2	34.781	68.206	31.328	1.00	96.21
	3241	O3	NAG	B	2	35.075	69.462	31.938	1.00	95.30
	3242	C4	NAG	B	2	35.966	67.760	30.458	1.00	94.75
	3243	O4	NAG	B	2	36.156	68.676	29.375	1.00	91.92
	3244	C5	NAG	B	2	35.704	66.327	29.921	1.00	95.52
	3245	O5	NAG	B	2	35.507	65.396	31.017	1.00	96.34
	3246	C6	NAG	B	2	36.873	65.825	29.101	1.00	96.13
	3247	O6	NAG	B	2	38.093	65.877	29.834	1.00	99.34
	3248	OH2	TIP	B	1	28.270	80.979	34.917	1.00	50.26
	3249	OH2	TIP	B	2	50.798	88.311	45.038	1.00	49.71
	3250	OH2	TIP	B	3	16.542	94.946	50.298	1.00	62.73
	3251	OH2	TIP	B	4	24.725	83.256	39.944	1.00	44.66
	3252	OH2	TIP	B	5	40.269	78.063	37.851	1.00	53.56
	3253	OH2	TIP	B	6	9.197	79.408	26.351	1.00	44.98
	3254	OH2	TIP	B	7	26.398	96.745	29.206	1.00	44.08
	3255	OH2	TIP	B	8	38.618	89.009	32.579	1.00	40.39
	3256	OH2	TIP	B	9	39.672	81.166	40.426	1.00	40.49
	3257	OH2	TIP	B	10	17.116	78.215	37.161	1.00	46.89

	3258	OH2	TIP	B	11	18.243	77.296	33.917	1.00	50.51
	3259	OH2	TIP	B	12	27.078	76.693	33.012	1.00	50.17
	3260	OH2	TIP	B	13	35.090	58.030	33.714	1.00	54.70
	3261	OH2	TIP	B	14	29.218	81.786	23.355	1.00	44.57
	3262	OH2	TIP	B	15	43.924	82.629	46.436	1.00	50.94
	3263	OH2	TIP	B	16	1.538	85.984	28.824	1.00	56.21
	3264	OH2	TIP	B	17	30.590	75.306	16.280	1.00	59.52
	3265	OH2	TIP	B	18	23.180	95.510	42.272	1.00	55.58
	3266	OH2	TIP	B	19	32.511	60.357	37.976	1.00	66.56
	3267	OH2	TIP	B	20	34.997	58.857	36.088	1.00	63.77
	3268	OH2	TIP	B	21	13.039	76.542	38.487	1.00	62.34
	3269	OH2	TIP	B	22	46.374	79.044	30.275	1.00	54.44
	3270	OH2	TIP	B	23	50.931	79.559	44.881	1.00	52.42
	3271	OH2	TIP	B	24	37.386	70.634	30.326	1.00	60.14
	3272	OH2	TIP	B	25	49.964	85.552	35.048	1.00	48.11
	3273	OH2	TIP	B	26	19.519	76.770	31.435	1.00	45.10
	3274	OH2	TIP	B	27	36.515	71.442	28.125	1.00	59.32
	3275	OH2	TIP	B	28	58.506	76.725	41.675	1.00	53.61
	3276	OH2	TIP	B	29	38.094	79.042	44.064	1.00	60.13
	3277	OH2	TIP	B	30	52.870	67.201	28.126	1.00	56.34
	3278	OH2	TIP	B	31	33.456	82.100	36.961	1.00	58.14
	3279	OH2	TIP	B	32	40.793	70.829	43.558	1.00	50.57
	3280	OH2	TIP	B	33	9.876	81.332	43.156	1.00	56.48
	3281	OH2	TIP	B	34	26.776	77.910	35.274	1.00	60.64
	3282	OH2	TIP	B	35	32.082	56.279	37.927	1.00	56.75
	3283	OH2	TIP	B	36	41.915	85.209	33.986	1.00	52.49
	3284	OH2	TIP	B	37	35.082	80.384	18.510	1.00	56.17
	3285	OH2	TIP	B	38	57.244	63.192	22.895	1.00	57.49
	3286	OH2	TIP	B	39	6.333	76.420	30.801	1.00	59.27
	3287	OH2	TIP	B	40	29.685	90.602	44.591	1.00	55.17
	3288	OH2	TIP	B	41	36.388	79.659	25.044	1.00	55.25
	3289	OH2	TIP	B	42	19.034	94.293	29.572	1.00	50.93
	3290	OH2	TIP	B	43	40.676	79.023	31.687	1.00	58.05
	3291	OH2	TIP	B	44	29.928	96.295	23.009	1.00	63.22
	3292	OH2	TIP	B	45	14.498	74.337	37.588	1.00	59.76
	3293	OH2	TIP	B	46	34.047	76.484	31.577	1.00	61.09
	3294	OH2	TIP	B	47	55.169	85.314	45.805	1.00	58.75
	3295	OH2	TIP	B	48	48.047	66.430	43.800	1.00	59.73
	3296	OH2	TIP	B	49	33.940	96.758	23.804	1.00	53.77
	3297	OH2	TIP	B	50	57.073	93.041	37.538	1.00	59.31
	3298	OH2	TIP	B	51	29.485	77.394	32.123	1.00	56.85
	3299	OH2	TIP	B	52	28.540	96.775	19.917	1.00	60.05
	3300	OH2	TIP	B	53	44.894	72.951	29.410	1.00	57.10
	3301	OH2	TIP	B	54	45.362	55.938	33.103	1.00	60.54
	3302	OH2	TIP	B	55	48.139	75.237	29.289	1.00	62.47
	3303	OH2	TIP	B	56	-1.034	81.059	27.240	1.00	64.33
	3304	OH2	TIP	B	57	35.432	94.188	20.969	1.00	52.42
	3305	OH2	TIP	B	58	17.286	95.575	43.504	1.00	60.20
	3306	OH2	TIP	B	59	41.972	83.557	20.901	1.00	59.26
	3307	OH2	TIP	B	60	29.469	59.186	40.661	1.00	62.09
	3308	OH2	TIP	B	61	51.530	82.833	43.577	1.00	65.16
	3309	OH2	TIP	B	62	26.641	90.990	45.263	1.00	59.85
	3310	OH2	TIP	B	63	46.399	87.498	46.342	1.00	56.88
	3311	OH2	TIP	B	64	25.335	75.984	42.835	1.00	53.06
	3312	OH2	TIP	B	65	8.193	87.217	28.036	1.00	60.26
	3313	OH2	TIP	B	66	28.032	88.745	44.846	1.00	59.03
	3314	OH2	TIP	B	67	40.713	72.843	34.794	1.00	54.95
	3315	OH2	TIP	B	68	8.183	78.374	34.568	1.00	57.65
	3316	OH2	TIP	B	69	38.121	88.788	17.047	1.00	59.41
	3317	OH2	TIP	B	70	40.671	93.547	43.325	1.00	62.27
	3318	OH2	TIP	B	71	31.413	68.974	32.122	1.00	55.86
	3319	OH2	TIP	B	72	51.257	72.484	46.323	1.00	59.39

	3320	OH2	TIP	B	73	30.484	83.899	40.314	1.00	59.25
	3321	OH2	TIP	B	74	55.561	71.680	37.852	1.00	53.17
	3322	OH2	TIP	B	75	53.223	94.913	42.289	1.00	65.55
	3323	OH2	TIP	B	76	55.467	63.809	25.190	1.00	62.05
	3324	OH2	TIP	B	77	31.319	66.997	30.418	1.00	57.87
	3325	OH2	TIP	B	78	29.297	94.140	18.414	1.00	58.31
	3326	OH2	TIP	B	79	9.882	83.094	29.532	1.00	53.97
	3327	OH2	TIP	B	80	55.788	84.688	33.186	1.00	54.45
	3328	OH2	TIP	B	81	14.402	84.006	43.396	1.00	60.50
	3329	OH2	TIP	B	82	21.401	99.644	31.527	1.00	54.25
	3330	OH2	TIP	B	83	38.747	99.305	29.133	1.00	58.03
	3331	OH2	TIP	B	84	36.701	91.635	49.414	1.00	61.54
	3332	OH2	TIP	B	85	53.184	73.221	55.411	1.00	71.84
	3333	OH2	TIP	B	86	54.962	57.175	32.829	1.00	59.92
	3334	OH2	TIP	B	87	37.795	94.920	41.465	1.00	55.82
	3335	OH2	TIP	B	88	47.047	68.720	45.430	1.00	57.31
	3336	OH2	TIP	B	89	53.386	88.730	45.407	1.00	58.45
	3337	OH2	TIP	B	90	12.966	80.192	43.065	1.00	58.03
	3338	OH2	TIP	B	91	25.222	92.505	24.772	1.00	50.36
	3339	OH2	TIP	B	92	56.971	75.837	46.165	1.00	57.19
	3340	OH2	TIP	B	93	52.883	57.456	41.616	1.00	62.27
	3341	OH2	TIP	B	94	21.647	72.884	37.586	1.00	61.49
	3342	OH2	TIP	B	95	53.819	55.355	36.996	1.00	66.72
	3343	OH2	TIP	B	96	1.978	86.114	32.124	1.00	62.93
	3344	OH2	TIP	B	97	3.673	88.829	34.679	1.00	59.08
	3345	OH2	TIP	B	98	50.288	52.210	35.596	1.00	66.54
	3346	OH2	TIP	B	99	53.869	54.763	33.809	1.00	64.16
	3347	OH2	TIP	B	100	39.796	81.619	49.309	1.00	59.09
	3348	OH2	TIP	B	101	27.537	82.048	39.451	1.00	59.99
	3349	OH2	TIP	B	102	36.131	103.395	30.948	1.00	63.48
	3350	OH2	TIP	B	103	56.043	76.714	32.065	1.00	60.94
	3351	OH2	TIP	B	104	31.838	89.133	20.071	1.00	57.13
	3352	OH2	TIP	B	105	49.027	92.881	29.882	1.00	67.01
	3353	OH2	TIP	B	106	52.660	69.955	44.183	1.00	61.12
	3354	OH2	TIP	B	107	57.992	83.903	35.849	1.00	62.98
	3355	OH2	TIP	B	108	35.733	75.725	27.339	1.00	63.30
	3356	OH2	TIP	B	109	40.575	98.578	26.825	1.00	57.78
	3357	OH2	TIP	B	110	47.643	81.928	28.944	1.00	65.34
	3358	OH2	TIP	B	111	5.312	87.158	27.438	1.00	56.09
	3359	OH2	TIP	B	112	49.841	88.326	23.196	1.00	62.75
	3360	OH2	TIP	B	113	6.598	93.132	35.325	1.00	58.88
	3361	OH2	TIP	B	114	27.092	100.653	31.174	1.00	63.28
	3362	OH2	TIP	B	115	42.024	53.749	39.435	1.00	65.61
	3363	OH2	TIP	B	116	50.539	76.914	27.922	1.00	60.98
	3364	OH2	TIP	B	117	47.538	92.256	33.656	1.00	60.98
	3365	OH2	TIP	B	118	5.166	74.252	29.209	1.00	58.25
	3366	OH2	TIP	B	119	38.217	72.245	31.919	1.00	55.29
	3367	OH2	TIP	B	120	32.252	55.236	35.199	1.00	56.80
	3368	OH2	TIP	B	121	32.670	57.598	33.803	1.00	61.15
	3369	OH2	TIP	B	122	17.786	96.981	50.771	1.00	55.82
	3370	OH2	TIP	B	123	40.380	77.020	40.041	1.00	45.14
	3371	OH2	TIP	B	124	42.038	88.110	33.725	1.00	55.49
	3372	OH2	TIP	B	125	34.758	55.495	34.823	1.00	66.22
	3373	OH2	TIP	B	126	37.737	77.084	41.644	1.00	57.00
	3374	OH2	TIP	B	127	29.699	98.301	28.668	1.00	57.60
	3375	OH2	TIP	B	128	49.020	89.370	46.224	1.00	56.82
	3376	OH2	TIP	B	129	52.859	75.885	25.996	1.00	62.05
	3377	OH2	TIP	B	130	30.010	59.209	36.597	1.00	66.31
	3378	OH2	TIP	B	131	30.914	96.977	25.231	1.00	57.71
	3379	OH2	TIP	B	132	39.916	79.723	47.627	1.00	61.64
	3380	OH2	TIP	B	133	44.108	57.405	44.718	1.00	61.06
	3381	OH2	TIP	B	134	9.863	79.457	23.833	1.00	61.78

	3382	OH2	TIP	B	135	38.917	86.317	18.760	1.00	57.35
	3383	OH2	TIP	B	136	30.862	81.856	35.179	1.00	54.03
	3384	OH2	TIP	B	137	53.704	70.947	53.894	1.00	64.00
	3385	OH2	TIP	B	138	40.859	81.838	22.227	1.00	65.85
	3386	OH2	TIP	B	139	37.816	96.128	20.409	1.00	60.91
	3387	OH2	TIP	B	140	25.705	74.474	33.305	1.00	61.62
	3388	OH2	TIP	B	141	30.005	54.298	36.646	1.00	62.13
	3389	OH2	TIP	B	142	10.624	79.976	28.177	1.00	58.14
	3390	OH2	TIP	B	143	29.498	59.385	43.076	1.00	61.05
	3391	OH2	TIP	B	144	40.320	90.895	16.086	1.00	55.65
	3392	OH2	TIP	B	145	55.724	66.531	26.778	1.00	64.64
	3393	OH2	TIP	B	146	50.659	94.738	31.683	1.00	61.54
	3394	OH2	TIP	B	147	3.656	85.417	24.832	1.00	59.07
	3395	OH2	TIP	B	148	16.265	75.893	38.242	1.00	60.79
	3396	OH2	TIP	B	149	31.777	95.407	41.590	1.00	57.59
	3397	OH2	TIP	B	150	54.287	76.248	53.590	1.00	63.92
	3398	OH2	TIP	B	151	33.491	79.601	16.793	1.00	62.67
	3399	OH2	TIP	B	152	19.155	94.756	51.118	1.00	68.07
	3400	OH2	TIP	B	153	35.245	75.050	34.131	1.00	61.87
	3401	OH2	TIP	B	154	56.335	76.647	34.751	1.00	66.95
	3402	OH2	TIP	B	155	55.588	94.784	38.616	1.00	59.56
	3403	OH2	TIP	B	156	36.064	78.257	16.816	1.00	59.20
	3404	OH2	TIP	B	157	55.289	57.324	36.670	1.00	67.18
	3405	OH2	TIP	B	158	38.244	95.684	44.137	1.00	59.37
	3406	OH2	TIP	B	159	-1.406	80.766	24.793	1.00	65.79
	3407	OH2	TIP	B	160	46.599	89.854	33.493	1.00	58.89
	3408	OH2	TIP	B	161	31.235	73.902	14.323	1.00	59.68
	3409	OH2	TIP	B	162	49.265	83.710	48.164	1.00	63.91
	3410	OH2	TIP	B	163	12.493	91.314	27.537	1.00	58.95
	3411	OH2	TIP	B	164	30.439	81.890	41.630	1.00	64.19
	3412	OH2	TIP	B	165	33.579	81.394	39.388	1.00	55.30
	3413	OH2	TIP	B	166	23.628	85.041	47.763	1.00	55.04
	3414	OH2	TIP	B	167	37.026	77.530	29.328	1.00	61.56
	3415	OH2	TIP	B	168	42.191	47.686	40.363	1.00	63.55
	3416	OH2	TIP	B	169	48.389	87.260	21.330	1.00	62.46
	3417	OH2	TIP	B	170	-1.110	78.818	28.205	1.00	61.28
	3418	OH2	TIP	B	171	30.316	77.346	15.355	1.00	59.15
	3419	OH2	TIP	B	172	56.892	58.723	34.712	1.00	66.69
	3420	OH2	TIP	B	173	38.573	89.823	51.022	1.00	60.64
	3421	OH2	TIP	B	174	55.700	73.403	29.957	1.00	64.56
	3422	OH2	TIP	B	175	2.131	82.160	29.752	1.00	59.77
	3423	OH2	TIP	B	176	48.652	75.463	25.876	1.00	61.95
	3424	OH2	TIP	B	177	13.930	79.132	45.787	1.00	63.68
	3425	OH2	TIP	B	178	49.048	79.772	28.026	1.00	62.71
	3426	OH2	TIP	B	179	50.873	71.018	26.463	1.00	64.40
	3427	OH2	TIP	B	180	-0.222	87.613	28.898	1.00	64.94
	3428	OH2	TIP	B	181	36.716	99.478	26.710	1.00	60.70
	3429	OH2	TIP	B	182	55.733	96.794	42.680	1.00	62.42
	3430	OH2	TIP	B	183	32.962	78.288	30.566	1.00	65.26
	3431	OH2	TIP	B	184	50.072	74.531	27.875	1.00	58.49
	3432	OH2	TIP	B	185	4.066	80.299	25.717	1.00	66.38
	3433	OH2	TIP	B	186	51.785	82.993	46.037	1.00	66.62
	3434	OH2	TIP	B	187	6.687	89.453	25.800	1.00	63.72
	3435	OH2	TIP	B	188	3.415	87.824	28.810	1.00	62.49
	3436	OH2	TIP	B	189	58.432	73.821	42.739	1.00	63.23
	3437	OH2	TIP	B	190	3.604	89.517	32.202	1.00	65.15
	3438	OH2	TIP	B	191	36.662	69.392	26.901	1.00	63.27
	3439	OH2	TIP	B	192	51.020	69.014	46.306	1.00	61.81
	3440	OH2	TIP	B	193	34.827	72.790	27.053	1.00	59.78
	3441	OH2	TIP	B	194	38.979	97.644	41.760	1.00	60.91
	3442	OH2	TIP	B	195	25.438	89.346	46.679	1.00	61.51

Another embodiment of the present invention is a 3-D model of a Fc-Cε3/Cε4 region that substantially represents the atomic coordinates specified (i.e., listed) in Table 2.

Table 2. Atomic coordinates of 1FP5_dimer.pdb

ATOM #	ATOM TYPE	RES	CHN	#	X	Y	Z	OCC	B
1	N	VAL	A	336	46.157	62.618	17.991	1.00	58.93
2	CA	VAL	A	336	45.400	61.812	16.993	1.00	60.44
3	C	VAL	A	336	44.013	61.427	17.501	1.00	60.07
4	O	VAL	A	336	43.847	60.389	18.142	1.00	61.48
5	CB	VAL	A	336	46.155	60.521	16.647	1.00	60.81
6	CG1	VAL	A	336	45.464	59.806	15.500	1.00	61.71
7	CG2	VAL	A	336	47.590	60.845	16.302	1.00	64.73
8	N	SER	A	337	43.017	62.257	17.209	1.00	57.95
9	CA	SER	A	337	41.655	61.983	17.648	1.00	56.60
10	C	SER	A	337	40.683	61.842	16.476	1.00	55.17
11	O	SER	A	337	40.981	62.262	15.352	1.00	54.55
12	CB	SER	A	337	41.185	63.078	18.603	1.00	57.92
13	OG	SER	A	337	41.489	64.356	18.087	1.00	64.70
14	N	ALA	A	338	39.527	61.238	16.743	1.00	52.40
15	CA	ALA	A	338	38.522	61.010	15.711	1.00	50.69
16	C	ALA	A	338	37.109	61.300	16.192	1.00	50.25
17	O	ALA	A	338	36.772	61.062	17.354	1.00	51.17
18	CB	ALA	A	338	38.611	59.573	15.211	1.00	50.21
19	N	TYR	A	339	36.281	61.808	15.284	1.00	48.22
20	CA	TYR	A	339	34.899	62.139	15.605	1.00	46.82
21	C	TYR	A	339	33.990	61.766	14.431	1.00	44.51
22	O	TYR	A	339	34.372	61.889	13.268	1.00	42.27
23	CB	TYR	A	339	34.765	63.638	15.915	1.00	50.52
24	CG	TYR	A	339	35.869	64.198	16.793	1.00	58.40
25	CD1	TYR	A	339	37.144	64.445	16.274	1.00	61.23
26	CD2	TYR	A	339	35.648	64.456	18.151	1.00	60.99
27	CE1	TYR	A	339	38.174	64.929	17.081	1.00	62.71
28	CE2	TYR	A	339	36.674	64.943	18.969	1.00	63.53
29	CZ	TYR	A	339	37.933	65.176	18.427	1.00	64.33
30	OH	TYR	A	339	38.953	65.644	19.230	1.00	65.07
31	N	LEU	A	340	32.793	61.291	14.746	1.00	41.90
32	CA	LEU	A	340	31.831	60.905	13.728	1.00	41.06
33	C	LEU	A	340	30.571	61.671	14.078	1.00	41.10
34	O	LEU	A	340	30.136	61.647	15.224	1.00	43.45
35	CB	LEU	A	340	31.583	59.392	13.779	1.00	36.93
36	CG	LEU	A	340	30.689	58.770	12.701	1.00	35.91
37	CD1	LEU	A	340	31.229	59.100	11.314	1.00	34.60
38	CD2	LEU	A	340	30.621	57.264	12.906	1.00	35.51
39	N	SER	A	341	29.990	62.368	13.108	1.00	39.82
40	CA	SER	A	341	28.790	63.152	13.385	1.00	39.85
41	C	SER	A	341	27.598	62.645	12.614	1.00	37.88
42	O	SER	A	341	27.737	62.076	11.544	1.00	42.10
43	CB	SER	A	341	29.025	64.627	13.042	1.00	39.34
44	OG	SER	A	341	29.347	64.792	11.672	1.00	44.58
45	N	ARG	A	342	26.415	62.868	13.158	1.00	36.98
46	CA	ARG	A	342	25.187	62.437	12.517	1.00	35.20
47	C	ARG	A	342	24.853	63.417	11.393	1.00	33.18
48	O	ARG	A	342	25.508	64.443	11.252	1.00	33.16
49	CB	ARG	A	342	24.070	62.394	13.566	1.00	38.57
50	CG	ARG	A	342	24.321	61.381	14.689	1.00	39.10
51	CD	ARG	A	342	23.191	61.364	15.712	1.00	43.21
52	NE	ARG	A	342	23.231	62.544	16.570	1.00	45.40

	53	CZ	ARG	A	342	24.086	62.714	17.573	1.00	48.22
	54	NH1	ARG	A	342	24.977	61.777	17.860	1.00	52.78
	55	NH2	ARG	A	342	24.059	63.831	18.286	1.00	54.34
	56	N	PRO	A	343	23.843	63.112	10.570	1.00	33.03
5	57	CA	PRO	A	343	23.497	64.040	9.481	1.00	34.14
	58	C	PRO	A	343	22.907	65.339	10.035	1.00	34.06
	59	O	PRO	A	343	22.302	65.341	11.106	1.00	35.44
	60	CB	PRO	A	343	22.448	63.266	8.667	1.00	33.07
	61	CG	PRO	A	343	22.700	61.811	9.025	1.00	35.06
10	62	CD	PRO	A	343	23.029	61.885	10.499	1.00	33.27
	63	N	SER	A	344	23.080	66.445	9.325	1.00	32.17
	64	CA	SER	A	344	22.490	67.691	9.792	1.00	31.75
	65	C	SER	A	344	21.014	67.617	9.414	1.00	32.07
	66	O	SER	A	344	20.660	67.115	8.344	1.00	30.21
15	67	CB	SER	A	344	23.144	68.907	9.118	1.00	32.20
	68	OG	SER	A	344	22.665	69.113	7.799	1.00	32.50
	69	N	PRO	A	345	20.127	68.088	10.300	1.00	32.31
	70	CA	PRO	A	345	18.701	68.039	9.975	1.00	30.84
	71	C	PRO	A	345	18.381	68.710	8.629	1.00	29.64
20	72	O	PRO	A	345	17.506	68.256	7.891	1.00	30.14
	73	CB	PRO	A	345	18.055	68.741	11.174	1.00	30.96
	74	CG	PRO	A	345	18.941	68.301	12.307	1.00	33.18
	75	CD	PRO	A	345	20.339	68.457	11.713	1.00	33.65
	76	N	PHE	A	346	19.103	69.769	8.292	1.00	28.34
25	77	CA	PHE	A	346	18.844	70.447	7.034	1.00	31.46
	78	C	PHE	A	346	19.085	69.522	5.831	1.00	32.46
	79	O	PHE	A	346	18.269	69.465	4.907	1.00	32.59
	80	CB	PHE	A	346	19.711	71.706	6.916	1.00	32.72
	81	CG	PHE	A	346	19.613	72.382	5.579	1.00	36.34
30	82	CD1	PHE	A	346	18.430	72.981	5.172	1.00	40.58
	83	CD2	PHE	A	346	20.702	72.411	4.722	1.00	36.76
	84	CE1	PHE	A	346	18.333	73.609	3.933	1.00	38.98
	85	CE2	PHE	A	346	20.615	73.037	3.482	1.00	40.15
	86	CZ	PHE	A	346	19.425	73.637	3.086	1.00	38.60
35	87	N	ASP	A	347	20.203	68.797	5.850	1.00	32.92
	88	CA	ASP	A	347	20.534	67.877	4.764	1.00	33.58
	89	C	ASP	A	347	19.555	66.704	4.733	1.00	34.26
	90	O	ASP	A	347	19.192	66.212	3.666	1.00	32.29
	91	CB	ASP	A	347	21.967	67.349	4.921	1.00	28.72
40	92	CG	ASP	A	347	23.008	68.364	4.521	1.00	39.62
	93	OD1	ASP	A	347	24.225	68.085	4.671	1.00	42.08
	94	OD2	ASP	A	347	22.609	69.449	4.046	1.00	46.23
	95	N	LEU	A	348	19.120	66.276	5.911	1.00	34.31
	96	CA	LEU	A	348	18.197	65.159	6.036	1.00	37.70
45	97	C	LEU	A	348	16.742	65.441	5.629	1.00	38.98
	98	O	LEU	A	348	16.137	64.651	4.902	1.00	38.11
	99	CB	LEU	A	348	18.220	64.641	7.482	1.00	40.66
	100	CG	LEU	A	348	17.333	63.441	7.840	1.00	41.99
	101	CD1	LEU	A	348	17.738	62.212	7.005	1.00	42.77
50	102	CD2	LEU	A	348	17.476	63.131	9.341	1.00	41.00
	103	N	PHE	A	349	16.183	66.560	6.083	1.00	39.68
	104	CA	PHE	A	349	14.781	66.875	5.794	1.00	42.09
	105	C	PHE	A	349	14.466	67.883	4.695	1.00	45.09
	106	O	PHE	A	349	13.431	67.779	4.038	1.00	48.27
55	107	CB	PHE	A	349	14.074	67.328	7.071	1.00	37.36
	108	CG	PHE	A	349	14.189	66.356	8.200	1.00	36.93
	109	CD1	PHE	A	349	15.021	66.624	9.282	1.00	38.16
	110	CD2	PHE	A	349	13.487	65.156	8.174	1.00	38.04
	111	CE1	PHE	A	349	15.155	65.715	10.319	1.00	38.11

	112	CE2	PHE	A	349	13.614	64.231	9.213	1.00	37.58
	113	CZ	PHE	A	349	14.449	64.511	10.283	1.00	40.39
	114	N	ILE	A	350	15.323	68.874	4.500	1.00	46.66
	115	CA	ILE	A	350	15.052	69.854	3.461	1.00	48.94
	116	C	ILE	A	350	15.695	69.400	2.150	1.00	51.15
	117	O	ILE	A	350	15.007	69.095	1.179	1.00	50.51
	118	CB	ILE	A	350	15.592	71.241	3.860	1.00	48.52
	119	CG1	ILE	A	350	15.172	71.562	5.299	1.00	49.25
	120	CG2	ILE	A	350	15.052	72.300	2.923	1.00	49.68
	121	CD1	ILE	A	350	13.689	71.358	5.567	1.00	46.80
	122	N	ARG	A	351	17.021	69.335	2.155	1.00	52.64
	123	CA	ARG	A	351	17.807	68.931	1.000	1.00	53.76
	124	C	ARG	A	351	17.510	67.486	0.581	1.00	53.61
	125	O	ARG	A	351	17.506	67.164	-0.603	1.00	53.55
	126	CB	ARG	A	351	19.287	69.095	1.341	1.00	56.64
	127	CG	ARG	A	351	20.166	69.584	0.206	1.00	62.18
	128	CD	ARG	A	351	21.225	70.527	0.752	1.00	66.96
	129	NE	ARG	A	351	22.389	70.642	-0.119	1.00	71.13
	130	CZ	ARG	A	351	23.229	69.643	-0.370	1.00	76.72
	131	NH1	ARG	A	351	23.027	68.455	0.184	1.00	78.73
	132	NH2	ARG	A	351	24.275	69.829	-1.168	1.00	77.63
	133	N	LYS	A	352	17.253	66.626	1.560	1.00	53.86
	134	CA	LYS	A	352	16.954	65.215	1.312	1.00	54.12
	135	C	LYS	A	352	18.151	64.428	0.772	1.00	52.02
	136	O	LYS	A	352	17.996	63.522	-0.046	1.00	51.77
	137	CB	LYS	A	352	15.775	65.075	0.347	1.00	57.77
	138	CG	LYS	A	352	14.476	65.689	0.846	1.00	62.15
	139	CD	LYS	A	352	13.348	65.439	-0.154	1.00	71.06
	140	CE	LYS	A	352	12.098	66.249	0.171	1.00	74.25
	141	NZ	LYS	A	352	12.293	67.707	-0.085	1.00	78.35
	142	N	SER	A	353	19.342	64.789	1.233	1.00	48.01
	143	CA	SER	A	353	20.568	64.112	0.832	1.00	45.29
	144	C	SER	A	353	21.544	64.154	2.016	1.00	40.67
	145	O	SER	A	353	22.546	64.875	1.994	1.00	40.76
	146	CB	SER	A	353	21.177	64.791	-0.398	1.00	47.97
	147	OG	SER	A	353	21.448	66.155	-0.147	1.00	56.20
	148	N	PRO	A	354	21.244	63.375	3.070	1.00	36.53
	149	CA	PRO	A	354	22.004	63.239	4.319	1.00	32.68
	150	C	PRO	A	354	23.399	62.660	4.139	1.00	31.88
	151	O	PRO	A	354	23.615	61.787	3.302	1.00	29.76
	152	CB	PRO	A	354	21.147	62.294	5.160	1.00	30.29
	153	CG	PRO	A	354	19.799	62.340	4.513	1.00	41.68
	154	CD	PRO	A	354	20.106	62.445	3.065	1.00	33.29
	155	N	THR	A	355	24.342	63.154	4.932	1.00	30.03
	156	CA	THR	A	355	25.704	62.644	4.902	1.00	29.70
	157	C	THR	A	355	26.236	62.578	6.326	1.00	30.82
	158	O	THR	A	355	25.773	63.298	7.213	1.00	30.67
	159	CB	THR	A	355	26.669	63.558	4.136	1.00	32.14
	160	OG1	THR	A	355	26.806	64.785	4.860	1.00	29.97
	161	CG2	THR	A	355	26.175	63.837	2.707	1.00	31.76
	162	N	ILE	A	356	27.195	61.693	6.558	1.00	30.53
	163	CA	ILE	A	356	27.816	61.631	7.868	1.00	31.56
	164	C	ILE	A	356	29.279	61.860	7.575	1.00	31.79
	165	O	ILE	A	356	29.752	61.561	6.475	1.00	30.35
	166	CB	ILE	A	356	27.584	60.285	8.583	1.00	30.05
	167	CG1	ILE	A	356	28.101	59.133	7.729	1.00	31.32
	168	CG2	ILE	A	356	26.092	60.131	8.890	1.00	31.27
	169	CD1	ILE	A	356	27.843	57.772	8.337	1.00	36.89
	170	N	THR	A	357	29.995	62.402	8.550	1.00	33.31
	171	CA	THR	A	357	31.395	62.719	8.349	1.00	33.68
	172	C	THR	A	357	32.282	62.197	9.456	1.00	35.47
	173	O	THR	A	357	31.993	62.372	10.641	1.00	36.65

	174	CB	THR	A	357	31.589	64.265	8.245	1.00	33.81
	175	OG1	THR	A	357	30.917	64.756	7.077	1.00	33.71
	176	CG2	THR	A	357	33.065	64.632	8.179	1.00	29.63
	177	N	CYS	A	358	33.372	61.566	9.052	1.00	35.41
	178	CA	CYS	A	358	34.346	61.039	9.990	1.00	38.12
	179	C	CYS	A	358	35.507	62.030	9.935	1.00	37.77
	180	O	CYS	A	358	36.127	62.205	8.890	1.00	36.67
	181	CB	CYS	A	358	34.811	59.655	9.532	1.00	40.37
	182	SG	CYS	A	358	35.831	58.729	10.726	1.00	49.83
	183	N	LEU	A	359	35.778	62.691	11.054	1.00	39.77
	184	CA	LEU	A	359	36.853	63.668	11.127	1.00	42.86
	185	C	LEU	A	359	38.007	63.168	11.977	1.00	46.01
	186	O	LEU	A	359	37.831	62.852	13.152	1.00	47.43
	187	CB	LEU	A	359	36.335	64.988	11.711	1.00	42.74
	188	CG	LEU	A	359	37.392	65.996	12.196	1.00	45.03
	189	CD1	LEU	A	359	38.262	66.448	11.043	1.00	47.59
	190	CD2	LEU	A	359	36.711	67.197	12.838	1.00	47.51
	191	N	VAL	A	360	39.189	63.107	11.379	1.00	48.26
	192	CA	VAL	A	360	40.380	62.669	12.090	1.00	52.34
	193	C	VAL	A	360	41.357	63.835	12.217	1.00	55.48
	194	O	VAL	A	360	41.672	64.508	11.234	1.00	55.57
	195	CB	VAL	A	360	41.073	61.500	11.353	1.00	53.36
	196	CG1	VAL	A	360	42.360	61.119	12.071	1.00	51.62
	197	CG2	VAL	A	360	40.133	60.301	11.284	1.00	51.77
	198	N	VAL	A	361	41.827	64.080	13.435	1.00	58.92
	199	CA	VAL	A	361	42.766	65.167	13.684	1.00	63.13
	200	C	VAL	A	361	44.094	64.607	14.174	1.00	67.77
	201	O	VAL	A	361	44.134	63.862	15.154	1.00	68.38
	202	CB	VAL	A	361	42.223	66.158	14.747	1.00	60.50
	203	CG1	VAL	A	361	43.245	67.242	15.014	1.00	56.92
	204	CG2	VAL	A	361	40.929	66.786	14.270	1.00	56.10
	205	N	ASP	A	362	45.174	64.965	13.485	1.00	72.90
	206	CA	ASP	A	362	46.515	64.502	13.841	1.00	78.30
	207	C	ASP	A	362	47.356	65.696	14.284	1.00	81.68
	208	O	ASP	A	362	47.891	66.432	13.452	1.00	81.72
	209	CB	ASP	A	362	47.185	63.829	12.638	1.00	80.22
	210	CG	ASP	A	362	48.444	63.070	13.020	1.00	84.67
	211	OD1	ASP	A	362	49.122	63.487	13.983	1.00	87.54
	212	OD2	ASP	A	362	48.763	62.063	12.351	1.00	87.19
	213	N	LEU	A	363	47.474	65.877	15.597	1.00	85.84
	214	CA	LEU	A	363	48.234	66.986	16.165	1.00	89.95
	215	C	LEU	A	363	49.677	67.038	15.672	1.00	92.20
	216	O	LEU	A	363	50.214	68.117	15.432	1.00	92.55
	217	CB	LEU	A	363	48.210	66.906	17.691	1.00	91.66
	218	CG	LEU	A	363	46.823	66.881	18.342	1.00	92.93
	219	CD1	LEU	A	363	46.976	66.787	19.854	1.00	95.41
	220	CD2	LEU	A	363	46.049	68.129	17.963	1.00	92.73
	221	N	ALA	A	364	50.304	65.874	15.527	1.00	94.76
	222	CA	ALA	A	364	51.684	65.799	15.049	1.00	97.66
	223	C	ALA	A	364	51.769	64.806	13.890	1.00	99.72
	224	O	ALA	A	364	51.604	63.602	14.079	1.00	100.44
	225	CB	ALA	A	364	52.604	65.365	16.179	1.00	97.99
	226	N	PRO	A	365	52.023	65.303	12.671	1.00	101.15
	227	CA	PRO	A	365	52.116	64.427	11.498	1.00	102.25
	228	C	PRO	A	365	53.437	63.705	11.245	1.00	103.43
	229	O	PRO	A	365	54.497	64.326	11.166	1.00	104.19
	230	CB	PRO	A	365	51.771	65.363	10.339	1.00	101.91
	231	CG	PRO	A	365	50.983	66.479	11.002	1.00	102.27
	232	CD	PRO	A	365	51.767	66.690	12.254	1.00	101.40
	233	N	SER	A	366	53.344	62.385	11.121	1.00	104.18
	234	CA	SER	A	366	54.468	61.512	10.801	1.00	104.43
	235	C	SER	A	366	53.924	61.027	9.463	1.00	104.05

	236	O	SER	A	366	52.736	60.712	9.373	1.00	104.36
	237	CB	SER	A	366	54.545	60.351	11.788	1.00	105.50
	238	OG	SER	A	366	53.377	59.560	11.687	1.00	106.70
	239	N	LYS	A	367	54.739	60.955	8.418	1.00	103.19
	240	CA	LYS	A	367	54.138	60.559	7.156	1.00	102.08
	241	C	LYS	A	367	53.970	59.109	6.733	1.00	100.74
	242	O	LYS	A	367	54.917	58.366	6.460	1.00	101.05
	243	CB	LYS	A	367	54.732	61.364	5.998	1.00	103.30
	244	CG	LYS	A	367	56.216	61.257	5.755	1.00	105.00
	245	CD	LYS	A	367	56.554	62.226	4.633	1.00	104.80
	246	CE	LYS	A	367	57.990	62.133	4.170	1.00	104.70
	247	NZ	LYS	A	367	58.214	63.076	3.034	1.00	105.18
	248	N	GLY	A	368	52.691	58.761	6.678	1.00	98.70
	249	CA	GLY	A	368	52.192	57.464	6.272	1.00	95.62
	250	C	GLY	A	368	50.799	57.900	5.856	1.00	93.12
	251	O	GLY	A	368	50.457	59.062	6.065	1.00	93.17
	252	N	THR	A	369	49.983	57.031	5.277	1.00	90.15
	253	CA	THR	A	369	48.652	57.475	4.880	1.00	86.41
	254	C	THR	A	369	47.623	57.180	5.964	1.00	83.04
	255	O	THR	A	369	47.746	56.198	6.699	1.00	82.54
	256	CB	THR	A	369	48.203	56.808	3.559	1.00	87.73
	257	OG1	THR	A	369	48.178	55.383	3.721	1.00	88.60
	258	CG2	THR	A	369	49.157	57.177	2.429	1.00	86.64
	259	N	VAL	A	370	46.620	58.048	6.073	1.00	79.07
	260	CA	VAL	A	370	45.559	57.871	7.058	1.00	74.46
	261	C	VAL	A	370	44.339	57.325	6.332	1.00	72.21
	262	O	VAL	A	370	43.762	57.998	5.482	1.00	71.35
	263	CB	VAL	A	370	45.180	59.199	7.732	1.00	73.33
	264	CG1	VAL	A	370	44.254	58.933	8.904	1.00	70.92
	265	CG2	VAL	A	370	46.427	59.926	8.185	1.00	69.77
	266	N	ASN	A	371	43.947	56.102	6.674	1.00	70.13
	267	CA	ASN	A	371	42.809	55.463	6.027	1.00	68.15
	268	C	ASN	A	371	41.521	55.443	6.838	1.00	65.65
	269	O	ASN	A	371	41.533	55.248	8.054	1.00	64.64
	270	CB	ASN	A	371	43.179	54.036	5.631	1.00	70.12
	271	CG	ASN	A	371	44.270	53.995	4.592	1.00	73.56
	272	OD1	ASN	A	371	44.081	54.447	3.462	1.00	75.10
	273	ND2	ASN	A	371	45.427	53.463	4.969	1.00	74.76
	274	N	LEU	A	372	40.408	55.651	6.141	1.00	62.66
	275	CA	LEU	A	372	39.088	55.641	6.754	1.00	59.53
	276	C	LEU	A	372	38.226	54.673	5.963	1.00	56.68
	277	O	LEU	A	372	38.071	54.812	4.753	1.00	56.70
	278	CB	LEU	A	372	38.459	57.040	6.728	1.00	59.44
	279	CG	LEU	A	372	39.217	58.172	7.422	1.00	60.55
	280	CD1	LEU	A	372	38.323	59.386	7.521	1.00	61.28
	281	CD2	LEU	A	372	39.644	57.739	8.807	1.00	62.83
	282	N	THR	A	373	37.669	53.689	6.654	1.00	53.76
	283	CA	THR	A	373	36.834	52.685	6.015	1.00	51.64
	284	C	THR	A	373	35.420	52.750	6.588	1.00	48.20
	285	O	THR	A	373	35.245	52.799	7.804	1.00	46.65
	286	CB	THR	A	373	37.399	51.275	6.268	1.00	53.15
	287	OG1	THR	A	373	38.811	51.276	6.027	1.00	57.77
	288	CG2	THR	A	373	36.729	50.261	5.353	1.00	53.75
	289	N	TRP	A	374	34.419	52.749	5.715	1.00	45.34
	290	CA	TRP	A	374	33.025	52.801	6.158	1.00	44.94
	291	C	TRP	A	374	32.341	51.439	6.059	1.00	43.68
	292	O	TRP	A	374	32.636	50.655	5.162	1.00	42.67
	293	CB	TRP	A	374	32.209	53.795	5.316	1.00	41.63
	294	CG	TRP	A	374	32.623	55.229	5.443	1.00	41.50
	295	CD1	TRP	A	374	33.476	55.912	4.623	1.00	39.67
	296	CD2	TRP	A	374	32.205	56.159	6.452	1.00	35.69
	297	NE1	TRP	A	374	33.612	57.208	5.059	1.00	35.06

	298	CE2	TRP	A	374	32.844	57.386	6.178	1.00	34.53
	299	CE3	TRP	A	374	31.353	56.072	7.558	1.00	32.37
	300	CZ2	TRP	A	374	32.657	58.521	6.971	1.00	35.43
	301	CZ3	TRP	A	374	31.166	57.199	8.349	1.00	36.11
	302	CH2	TRP	A	374	31.818	58.410	8.050	1.00	37.51
	303	N	SER	A	375	31.421	51.170	6.981	1.00	43.53
	304	CA	SER	A	375	30.666	49.922	6.960	1.00	43.57
	305	C	SER	A	375	29.330	50.089	7.662	1.00	42.59
	306	O	SER	A	375	29.189	50.931	8.550	1.00	43.68
	307	CB	SER	A	375	31.447	48.780	7.626	1.00	45.03
	308	OG	SER	A	375	31.482	48.909	9.034	1.00	45.66
	309	N	ARG	A	376	28.349	49.301	7.234	1.00	40.79
	310	CA	ARG	A	376	27.031	49.321	7.834	1.00	40.12
	311	C	ARG	A	376	26.911	48.102	8.749	1.00	40.59
	312	O	ARG	A	376	27.207	46.982	8.348	1.00	40.90
	313	CB	ARG	A	376	25.947	49.255	6.766	1.00	40.03
	314	CG	ARG	A	376	25.855	50.468	5.863	1.00	43.20
	315	CD	ARG	A	376	24.402	50.717	5.501	1.00	41.05
	316	NE	ARG	A	376	24.120	50.429	4.108	1.00	50.71
	317	CZ	ARG	A	376	22.895	50.300	3.612	1.00	53.97
	318	NH1	ARG	A	376	21.842	50.428	4.407	1.00	51.88
	319	NH2	ARG	A	376	22.726	50.058	2.318	1.00	55.55
	320	N	ALA	A	377	26.471	48.319	9.978	1.00	40.20
	321	CA	ALA	A	377	26.327	47.218	10.919	1.00	40.25
	322	C	ALA	A	377	25.470	46.100	10.314	1.00	40.38
	323	O	ALA	A	377	25.621	44.943	10.678	1.00	41.16
	324	CB	ALA	A	377	25.697	47.721	12.222	1.00	33.12
	325	N	SER	A	378	24.585	46.456	9.386	1.00	40.21
	326	CA	SER	A	378	23.697	45.491	8.746	1.00	41.95
	327	C	SER	A	378	24.412	44.694	7.664	1.00	44.92
	328	O	SER	A	378	23.856	43.734	7.134	1.00	44.28
	329	CB	SER	A	378	22.504	46.199	8.108	1.00	40.91
	330	OG	SER	A	378	22.907	46.863	6.920	1.00	40.09
	331	N	GLY	A	379	25.633	45.107	7.332	1.00	46.93
	332	CA	GLY	A	379	26.405	44.419	6.313	1.00	49.77
	333	C	GLY	A	379	26.088	44.884	4.904	1.00	50.60
	334	O	GLY	A	379	26.817	44.576	3.958	1.00	52.95
	335	N	LYS	A	380	24.995	45.626	4.755	1.00	53.72
	336	CA	LYS	A	380	24.612	46.122	3.443	1.00	54.13
	337	C	LYS	A	380	25.689	47.036	2.845	1.00	48.16
	338	O	LYS	A	380	26.592	47.513	3.544	1.00	45.65
	339	CB	LYS	A	380	23.262	46.848	3.517	1.00	62.44
	340	CG	LYS	A	380	22.078	45.908	3.710	1.00	67.72
	341	CD	LYS	A	380	20.748	46.625	3.550	1.00	69.32
	342	CE	LYS	A	380	19.587	45.644	3.619	1.00	73.14
	343	NZ	LYS	A	380	18.267	46.320	3.467	1.00	77.37
	344	N	PRO	A	381	25.614	47.277	1.529	1.00	56.07
	345	CA	PRO	A	381	26.586	48.128	0.835	1.00	56.46
	346	C	PRO	A	381	26.535	49.607	1.225	1.00	54.32
	347	O	PRO	A	381	25.467	50.154	1.511	1.00	56.76
	348	CB	PRO	A	381	26.225	47.936	-0.640	1.00	60.70
	349	CG	PRO	A	381	25.481	46.622	-0.667	1.00	62.01
	350	CD	PRO	A	381	24.655	46.695	0.574	1.00	59.24
	351	N	VAL	A	382	27.701	50.244	1.234	1.00	55.74
	352	CA	VAL	A	382	27.795	51.669	1.531	1.00	55.58
	353	C	VAL	A	382	28.192	52.353	0.220	1.00	55.56
	354	O	VAL	A	382	28.866	51.752	-0.620	1.00	55.22
	355	CB	VAL	A	382	28.874	51.980	2.607	1.00	55.39
	356	CG1	VAL	A	382	28.592	51.196	3.878	1.00	55.94
	357	CG2	VAL	A	382	30.261	51.664	2.075	1.00	53.06
	358	N	ASN	A	383	27.773	53.600	0.045	1.00	54.38
	359	CA	ASN	A	383	28.090	54.354	-1.164	1.00	54.63

	360	C	ASN	A	383	29.532	54.843	-1.190	1.00	53.85
	361	O	ASN	A	383	30.303	54.630	-0.254	1.00	52.58
	362	CB	ASN	A	383	27.171	55.566	-1.282	1.00	59.07
	363	CG	ASN	A	383	25.717	55.186	-1.356	1.00	64.60
	364	OD1	ASN	A	383	24.836	56.024	-1.169	1.00	70.14
	365	ND2	ASN	A	383	25.450	53.915	-1.638	1.00	71.07
	366	N	HIS	A	384	29.890	55.506	-2.281	1.00	53.46
	367	CA	HIS	A	384	31.229	56.057	-2.426	1.00	52.22
	368	C	HIS	A	384	31.326	57.302	-1.540	1.00	49.10
	369	O	HIS	A	384	30.400	58.105	-1.485	1.00	45.53
	370	CB	HIS	A	384	31.489	56.417	-3.893	1.00	59.11
	371	CG	HIS	A	384	31.676	55.223	-4.778	1.00	62.16
	372	ND1	HIS	A	384	32.738	54.357	-4.639	1.00	69.15
	373	CD2	HIS	A	384	30.931	54.745	-5.803	1.00	70.28
	374	CE1	HIS	A	384	32.640	53.394	-5.539	1.00	75.01
	375	NE2	HIS	A	384	31.553	53.605	-6.258	1.00	74.58
	376	N	SER	A	385	32.448	57.454	-0.849	1.00	45.07
	377	CA	SER	A	385	32.641	58.583	0.040	1.00	44.61
	378	C	SER	A	385	33.617	59.627	-0.504	1.00	44.58
	379	O	SER	A	385	34.380	59.356	-1.421	1.00	44.21
	380	CB	SER	A	385	33.113	58.076	1.409	1.00	44.61
	381	CG	SER	A	385	34.293	57.290	1.311	1.00	41.13
	382	N	THR	A	386	33.575	60.827	0.065	1.00	44.32
	383	CA	THR	A	386	34.450	61.916	-0.346	1.00	44.35
	384	C	THR	A	386	35.487	62.156	0.737	1.00	44.09
	385	O	THR	A	386	35.149	62.326	1.911	1.00	44.06
	386	CB	THR	A	386	33.664	63.226	-0.580	1.00	45.20
	387	OG1	THR	A	386	32.744	63.045	-1.662	1.00	51.89
	388	CG2	THR	A	386	34.616	64.368	-0.936	1.00	47.20
	389	N	ARG	A	387	36.749	62.176	0.326	1.00	44.39
	390	CA	ARG	A	387	37.870	62.378	1.233	1.00	46.68
	391	C	ARG	A	387	38.520	63.763	1.070	1.00	47.05
	392	O	ARG	A	387	38.750	64.228	-0.049	1.00	46.65
	393	CB	ARG	A	387	38.906	61.284	0.979	1.00	48.13
	394	CG	ARG	A	387	40.112	61.330	1.890	1.00	52.77
	395	CD	ARG	A	387	41.247	60.494	1.320	1.00	56.60
	396	NE	ARG	A	387	42.459	60.622	2.121	1.00	60.65
	397	CZ	ARG	A	387	42.705	59.917	3.218	1.00	61.97
	398	NH1	ARG	A	387	41.821	59.022	3.636	1.00	64.45
	399	NH2	ARG	A	387	43.819	60.131	3.911	1.00	60.54
	400	N	LYS	A	388	38.820	64.415	2.190	1.00	46.93
	401	CA	LYS	A	388	39.457	65.730	2.167	1.00	47.51
	402	C	LYS	A	388	40.630	65.777	3.143	1.00	48.33
	403	O	LYS	A	388	40.493	65.401	4.306	1.00	46.08
	404	CB	LYS	A	388	38.452	66.823	2.537	1.00	46.64
	405	CG	LYS	A	388	37.274	66.909	1.603	1.00	52.75
	406	CD	LYS	A	388	36.154	67.739	2.195	1.00	58.62
	407	CE	LYS	A	388	34.863	67.538	1.418	1.00	62.49
	408	NZ	LYS	A	388	33.719	68.204	2.101	1.00	67.33
	409	N	GLU	A	389	41.780	66.236	2.651	1.00	50.07
	410	CA	GLU	A	389	42.998	66.357	3.454	1.00	51.86
	411	C	GLU	A	389	43.474	67.807	3.462	1.00	52.81
	412	O	GLU	A	389	43.683	68.408	2.405	1.00	49.21
	413	CB	GLU	A	389	44.106	65.474	2.877	1.00	54.67
	414	CG	GLU	A	389	43.890	63.984	3.056	1.00	65.65
	415	CD	GLU	A	389	44.992	63.159	2.412	1.00	72.66
	416	OE1	GLU	A	389	46.182	63.449	2.671	1.00	75.92
	417	OE2	GLU	A	389	44.669	62.220	1.650	1.00	75.78
	418	N	GLU	A	390	43.652	68.371	4.651	1.00	56.06
	419	CA	GLU	A	390	44.100	69.751	4.754	1.00	61.17
	420	C	GLU	A	390	45.146	69.971	5.835	1.00	64.70
	421	O	GLU	A	390	45.002	69.528	6.977	1.00	64.01

	422	CB	GLU	A	390	42.908	70.673	4.993	1.00	64.35
	423	CG	GLU	A	390	43.283	72.121	5.233	1.00	74.80
	424	CD	GLU	A	390	42.091	73.052	5.121	1.00	85.97
	425	OE1	GLU	A	390	41.053	72.778	5.764	1.00	92.60
	426	OE2	GLU	A	390	42.197	74.059	4.388	1.00	92.18
	427	N	LYS	A	391	46.204	70.679	5.461	1.00	68.18
	428	CA	LYS	A	391	47.288	70.960	6.388	1.00	71.58
	429	C	LYS	A	391	47.298	72.385	6.920	1.00	76.11
	430	O	LYS	A	391	46.927	73.335	6.231	1.00	75.89
	431	CB	LYS	A	391	48.627	70.654	5.728	1.00	67.28
	432	N	GLN	A	392	47.724	72.508	8.168	1.00	81.85
	433	CA	GLN	A	392	47.854	73.786	8.846	1.00	88.38
	434	C	GLN	A	392	49.118	73.574	9.657	1.00	92.30
	435	O	GLN	A	392	49.100	72.848	10.648	1.00	93.25
	436	CB	GLN	A	392	46.662	74.045	9.777	1.00	85.87
	437	CG	GLN	A	392	45.752	75.178	9.318	1.00	90.76
	438	CD	GLN	A	392	44.727	75.573	10.369	1.00	93.39
	439	OE1	GLN	A	392	45.076	75.913	11.502	1.00	92.93
	440	NE2	GLN	A	392	43.453	75.538	9.993	1.00	93.97
	441	N	ARG	A	393	50.221	74.174	9.220	1.00	96.24
	442	CA	ARG	A	393	51.492	74.011	9.916	1.00	100.53
	443	C	ARG	A	393	51.412	74.350	11.403	1.00	102.30
	444	O	ARG	A	393	52.422	74.327	12.107	1.00	101.15
	445	CB	ARG	A	393	52.579	74.853	9.245	1.00	106.99
	446	CG	ARG	A	393	52.404	76.349	9.396	1.00	109.77
	447	CD	ARG	A	393	53.493	77.079	8.636	1.00	115.73
	448	NE	ARG	A	393	53.515	78.505	8.935	1.00	119.73
	449	CZ	ARG	A	393	54.333	79.373	8.350	1.00	121.60
	450	NH1	ARG	A	393	55.194	78.955	7.430	1.00	121.59
	451	NH2	ARG	A	393	54.292	80.655	8.684	1.00	121.49
	452	N	ASN	A	394	50.209	74.658	11.876	1.00	103.98
	453	CA	ASN	A	394	50.005	74.970	13.281	1.00	106.60
	454	C	ASN	A	394	50.275	73.682	14.051	1.00	106.89
	455	O	ASN	A	394	51.084	73.650	14.978	1.00	108.55
	456	CB	ASN	A	394	48.564	75.427	13.520	1.00	108.97
	457	CG	ASN	A	394	48.326	75.891	14.947	1.00	112.83
	458	OD1	ASN	A	394	47.190	76.141	15.348	1.00	114.53
	459	ND2	ASN	A	394	49.402	76.016	15.719	1.00	114.40
	460	N	GLY	A	395	49.593	72.616	13.648	1.00	105.53
	461	CA	GLY	A	395	49.771	71.331	14.298	1.00	101.15
	462	C	GLY	A	395	48.585	70.423	14.050	1.00	97.82
	463	O	GLY	A	395	48.125	69.721	14.952	1.00	99.41
	464	N	THR	A	396	48.084	70.423	12.822	1.00	94.50
	465	CA	THR	A	396	46.937	69.589	12.522	1.00	89.02
	466	C	THR	A	396	46.763	69.174	11.071	1.00	83.93
	467	O	THR	A	396	46.477	70.000	10.204	1.00	83.27
	468	CB	THR	A	396	45.625	70.278	12.970	1.00	92.03
	469	OG1	THR	A	396	45.648	70.484	14.388	1.00	94.17
	470	CG2	THR	A	396	44.414	69.421	12.596	1.00	95.48
	471	N	LEU	A	397	46.942	67.882	10.821	1.00	79.69
	472	CA	LEU	A	397	46.729	67.320	9.500	1.00	74.75
	473	C	LEU	A	397	45.295	66.827	9.604	1.00	71.50
	474	O	LEU	A	397	45.052	65.720	10.081	1.00	74.81
	475	CB	LEU	A	397	47.640	66.120	9.240	1.00	75.72
	476	CG	LEU	A	397	47.188	65.250	8.053	1.00	70.67
	477	CD1	LEU	A	397	47.668	65.858	6.738	1.00	69.05
	478	CD2	LEU	A	397	47.723	63.832	8.213	1.00	72.96
	479	N	THR	A	398	44.348	67.659	9.195	1.00	67.61
	480	CA	THR	A	398	42.945	67.286	9.252	1.00	61.30
	481	C	THR	A	398	42.559	66.393	8.076	1.00	56.61
	482	O	THR	A	398	42.960	66.626	6.934	1.00	54.95
	483	CB	THR	A	398	42.044	68.530	9.248	1.00	61.75

	484	OG1	THR	A	398	42.225	69.255	10.471	1.00	65.40
	485	CG2	THR	A	398	40.584	68.129	9.108	1.00	63.39
	486	N	VAL	A	399	41.783	65.359	8.371	1.00	51.84
	487	CA	VAL	A	399	41.321	64.437	7.349	1.00	48.05
	488	C	VAL	A	399	39.870	64.085	7.610	1.00	44.81
	489	O	VAL	A	399	39.502	63.689	8.719	1.00	44.41
	490	CB	VAL	A	399	42.132	63.134	7.349	1.00	49.35
	491	CG1	VAL	A	399	41.590	62.191	6.295	1.00	49.43
	492	CG2	VAL	A	399	43.594	63.432	7.090	1.00	53.10
	493	N	THR	A	400	39.036	64.246	6.596	1.00	42.44
	494	CA	THR	A	400	37.635	63.909	6.757	1.00	40.44
	495	C	THR	A	400	37.151	63.068	5.602	1.00	38.07
	496	O	THR	A	400	37.692	63.117	4.498	1.00	36.13
	497	CB	THR	A	400	36.731	65.152	6.834	1.00	39.64
	498	OG1	THR	A	400	36.638	65.755	5.539	1.00	43.72
	499	CG2	THR	A	400	37.278	66.158	7.822	1.00	38.32
	500	N	SER	A	401	36.140	62.265	5.884	1.00	36.90
	501	CA	SER	A	401	35.531	61.432	4.876	1.00	35.46
	502	C	SER	A	401	34.043	61.612	5.084	1.00	33.95
	503	O	SER	A	401	33.538	61.447	6.192	1.00	34.80
	504	CB	SER	A	401	35.906	59.962	5.060	1.00	36.91
	505	OG	SER	A	401	35.299	59.183	4.040	1.00	40.84
	506	N	THR	A	402	33.352	61.965	4.014	1.00	32.28
	507	CA	THR	A	402	31.928	62.178	4.068	1.00	31.85
	508	C	THR	A	402	31.245	61.092	3.264	1.00	31.76
	509	O	THR	A	402	31.554	60.863	2.090	1.00	30.55
	510	CB	THR	A	402	31.570	63.549	3.505	1.00	31.33
	511	OG1	THR	A	402	32.284	64.542	4.238	1.00	32.83
	512	CG2	THR	A	402	30.078	63.818	3.632	1.00	32.70
	513	N	LEU	A	403	30.299	60.433	3.912	1.00	30.72
	514	CA	LEU	A	403	29.582	59.343	3.300	1.00	30.33
	515	C	LEU	A	403	28.115	59.673	3.097	1.00	29.66
	516	O	LEU	A	403	27.415	59.992	4.052	1.00	28.06
	517	CB	LEU	A	403	29.698	58.098	4.187	1.00	28.34
	518	CG	LEU	A	403	28.968	56.831	3.719	1.00	32.10
	519	CD1	LEU	A	403	29.777	56.175	2.597	1.00	31.94
	520	CD2	LEU	A	403	28.810	55.844	4.876	1.00	30.42
	521	N	PRO	A	404	27.638	59.617	1.841	1.00	31.48
	522	CA	PRO	A	404	26.233	59.896	1.534	1.00	33.20
	523	C	PRO	A	404	25.451	58.759	2.194	1.00	34.02
	524	O	PRO	A	404	25.845	57.601	2.104	1.00	32.25
	525	CB	PRO	A	404	26.183	59.812	0.010	1.00	33.28
	526	CG	PRO	A	404	27.590	60.165	-0.400	1.00	31.82
	527	CD	PRO	A	404	28.413	59.414	0.603	1.00	31.26
	528	N	VAL	A	405	24.362	59.097	2.865	1.00	34.94
	529	CA	VAL	A	405	23.556	58.117	3.564	1.00	38.63
	530	C	VAL	A	405	22.128	58.059	3.032	1.00	40.02
	531	O	VAL	A	405	21.573	59.063	2.598	1.00	40.31
	532	CB	VAL	A	405	23.548	58.457	5.082	1.00	42.09
	533	CG1	VAL	A	405	22.128	58.490	5.632	1.00	43.95
	534	CG2	VAL	A	405	24.405	57.456	5.827	1.00	41.76
	535	N	GLY	A	406	21.536	56.872	3.061	1.00	42.35
	536	CA	GLY	A	406	20.168	56.741	2.597	1.00	43.35
	537	C	GLY	A	406	19.246	57.422	3.587	1.00	43.87
	538	O	GLY	A	406	19.446	57.314	4.797	1.00	42.68
	539	N	THR	A	407	18.248	58.134	3.077	1.00	44.40
	540	CA	THR	A	407	17.294	58.840	3.923	1.00	47.37
	541	C	THR	A	407	16.473	57.887	4.778	1.00	48.27
	542	O	THR	A	407	16.392	58.051	5.993	1.00	48.77
	543	CB	THR	A	407	16.312	59.678	3.078	1.00	48.44
	544	OG1	THR	A	407	17.001	60.791	2.504	1.00	50.00
	545	CG2	THR	A	407	15.164	60.187	3.938	1.00	53.23

	546	N	ARG	A	408	15.854	56.903	4.130	1.00	48.10
55	547	CA	ARG	A	408	15.021	55.935	4.821	1.00	48.54
	548	C	ARG	A	408	15.827	55.060	5.765	1.00	48.48
	549	O	ARG	A	408	15.418	54.831	6.903	1.00	47.34
	550	CB	ARG	A	408	14.275	55.070	3.810	1.00	50.16
	551	N	ASP	A	409	16.966	54.567	5.294	1.00	48.72
5	552	CA	ASP	A	409	17.813	53.714	6.121	1.00	50.88
	553	C	ASP	A	409	18.179	54.413	7.426	1.00	49.92
	554	O	ASP	A	409	18.132	53.811	8.502	1.00	49.76
	555	CB	ASP	A	409	19.088	53.340	5.362	1.00	56.18
	556	CG	ASP	A	409	18.799	52.587	4.074	1.00	64.80
10	557	OD1	ASP	A	409	18.118	51.538	4.144	1.00	71.41
	558	OD2	ASP	A	409	19.247	53.039	2.995	1.00	68.29
	559	N	TRP	A	410	18.533	55.692	7.327	1.00	48.36
	560	CA	TRP	A	410	18.914	56.458	8.503	1.00	46.32
	561	C	TRP	A	410	17.736	56.647	9.447	1.00	46.21
15	562	O	TRP	A	410	17.869	56.489	10.660	1.00	44.64
	563	CB	TRP	A	410	19.480	57.826	8.108	1.00	42.82
	564	CG	TRP	A	410	19.890	58.599	9.304	1.00	39.31
	565	CD1	TRP	A	410	19.133	59.496	9.997	1.00	37.29
	566	CD2	TRP	A	410	21.093	58.419	10.057	1.00	35.49
20	567	NE1	TRP	A	410	19.781	59.874	11.143	1.00	39.24
	568	CE2	TRP	A	410	20.987	59.228	11.205	1.00	32.76
	569	CE3	TRP	A	410	22.249	57.644	9.872	1.00	32.07
	570	CZ2	TRP	A	410	21.994	59.291	12.176	1.00	29.59
	571	CZ3	TRP	A	410	23.248	57.704	10.831	1.00	33.68
25	572	CH2	TRP	A	410	23.111	58.527	11.975	1.00	30.56
	573	N	ILE	A	411	16.584	56.989	8.888	1.00	48.11
	574	CA	ILE	A	411	15.391	57.192	9.699	1.00	50.90
	575	C	ILE	A	411	14.951	55.888	10.358	1.00	52.46
	576	O	ILE	A	411	14.371	55.902	11.442	1.00	53.34
30	577	CB	ILE	A	411	14.234	57.755	8.854	1.00	51.58
	578	CG1	ILE	A	411	14.613	59.144	8.330	1.00	52.81
	579	CG2	ILE	A	411	12.966	57.828	9.685	1.00	51.95
	580	CD1	ILE	A	411	13.566	59.777	7.431	1.00	59.38
	581	N	GLU	A	412	15.252	54.763	9.715	1.00	53.21
35	582	CA	GLU	A	412	14.872	53.463	10.248	1.00	53.12
	583	C	GLU	A	412	15.853	52.919	11.269	1.00	51.24
	584	O	GLU	A	412	15.610	51.864	11.848	1.00	51.40
	585	CB	GLU	A	412	14.691	52.448	9.119	1.00	59.71
	586	CG	GLU	A	412	13.362	52.578	8.383	1.00	70.52
40	587	CD	GLU	A	412	13.201	51.540	7.290	1.00	78.58
	588	OE1	GLU	A	412	13.402	50.338	7.573	1.00	83.44
	589	OE2	GLU	A	412	12.868	51.924	6.150	1.00	82.10
	590	N	GLY	A	413	16.966	53.618	11.477	1.00	48.47
	591	CA	GLY	A	413	17.923	53.173	12.474	1.00	44.62
45	592	C	GLY	A	413	19.213	52.484	12.068	1.00	44.15
	593	O	GLY	A	413	19.882	51.913	12.927	1.00	43.50
	594	N	GLU	A	414	19.588	52.515	10.793	1.00	42.78
	595	CA	GLU	A	414	20.843	51.878	10.406	1.00	40.78
	596	C	GLU	A	414	21.948	52.495	11.249	1.00	39.97
50	597	O	GLU	A	414	21.842	53.645	11.690	1.00	37.43
	598	CB	GLU	A	414	21.155	52.111	8.918	1.00	41.96
	599	CG	GLU	A	414	22.519	51.566	8.441	1.00	44.09
	600	CD	GLU	A	414	22.582	50.036	8.360	1.00	49.01
	601	OE1	GLU	A	414	23.051	49.387	9.325	1.00	46.84
55	602	OE2	GLU	A	414	22.152	49.479	7.327	1.00	49.89
	603	N	THR	A	415	23.001	51.721	11.485	1.00	39.56

	604	CA	THR	A	415	24.136	52.197	12.253	1.00	40.76
	605	C	THR	A	415	25.369	52.113	11.362	1.00	40.07
	606	O	THR	A	415	25.640	51.067	10.777	1.00	42.10
	607	CB	THR	A	415	24.327	51.362	13.544	1.00	44.69
	608	OG1	THR	A	415	25.707	51.378	13.929	1.00	51.98
	609	CG2	THR	A	415	23.856	49.948	13.342	1.00	50.00
	610	N	TYR	A	416	26.100	53.220	11.240	1.00	37.57
	611	CA	TYR	A	416	27.282	53.273	10.386	1.00	34.50
	612	C	TYR	A	416	28.549	53.335	11.201	1.00	36.77
	613	O	TYR	A	416	28.562	53.894	12.300	1.00	35.94
	614	CB	TYR	A	416	27.221	54.484	9.466	1.00	34.15
	615	CG	TYR	A	416	26.003	54.515	8.586	1.00	30.65
	616	CD1	TYR	A	416	24.744	54.823	9.108	1.00	32.53
	617	CD2	TYR	A	416	26.101	54.211	7.235	1.00	31.72
	618	CE1	TYR	A	416	23.616	54.828	8.297	1.00	34.27
	619	CE2	TYR	A	416	24.981	54.210	6.420	1.00	32.11
	620	CZ	TYR	A	416	23.744	54.520	6.956	1.00	33.86
	621	OH	TYR	A	416	22.636	54.518	6.139	1.00	41.22
	622	N	GLN	A	417	29.624	52.771	10.659	1.00	37.58
	623	CA	GLN	A	417	30.878	52.752	11.386	1.00	39.43
	624	C	GLN	A	417	32.062	53.259	10.582	1.00	39.40
	625	O	GLN	A	417	32.227	52.936	9.406	1.00	39.63
	626	CB	GLN	A	417	31.179	51.331	11.889	1.00	41.37
	627	CG	GLN	A	417	32.386	51.250	12.822	1.00	51.81
	628	CD	GLN	A	417	32.744	49.827	13.214	1.00	61.69
	629	OE1	GLN	A	417	33.229	49.045	12.390	1.00	67.15
	630	NE2	GLN	A	417	32.504	49.481	14.479	1.00	63.64
	631	N	CYS	A	418	32.888	54.057	11.236	1.00	39.29
	632	CA	CYS	A	418	34.083	54.581	10.611	1.00	41.80
	633	C	CYS	A	418	35.250	53.880	11.282	1.00	42.50
	634	O	CYS	A	418	35.409	53.954	12.500	1.00	43.33
	635	CB	CYS	A	418	34.208	56.099	10.825	1.00	41.95
	636	SG	CYS	A	418	35.696	56.805	10.043	1.00	54.15
	637	N	ARG	A	419	36.049	53.182	10.491	1.00	43.98
	638	CA	ARG	A	419	37.225	52.497	11.007	1.00	47.51
	639	C	ARG	A	419	38.428	53.323	10.558	1.00	48.11
	640	O	ARG	A	419	38.741	53.381	9.370	1.00	47.85
	641	CB	ARG	A	419	37.289	51.068	10.452	1.00	49.08
	642	CG	ARG	A	419	38.642	50.397	10.586	1.00	54.11
	643	CD	ARG	A	419	38.554	48.892	10.304	1.00	64.71
	644	NE	ARG	A	419	39.868	48.275	10.137	1.00	64.09
	645	CZ	ARG	A	419	40.493	48.163	8.968	1.00	70.31
	646	NH1	ARG	A	419	39.919	48.619	7.861	1.00	68.32
	647	NH2	ARG	A	419	41.699	47.608	8.905	1.00	71.53
	648	N	VAL	A	420	39.076	53.990	11.508	1.00	51.04
	649	CA	VAL	A	420	40.231	54.824	11.200	1.00	56.22
	650	C	VAL	A	420	41.532	54.039	11.354	1.00	61.25
	651	O	VAL	A	420	41.780	53.422	12.393	1.00	60.11
	652	CB	VAL	A	420	40.295	56.064	12.115	1.00	54.44
	653	CG1	VAL	A	420	41.494	56.922	11.729	1.00	52.69
	654	CG2	VAL	A	420	39.003	56.868	12.005	1.00	55.45
	655	N	THR	A	421	42.359	54.071	10.314	1.00	66.23
	656	CA	THR	A	421	43.631	53.356	10.326	1.00	73.18
	657	C	THR	A	421	44.834	54.266	10.130	1.00	76.87
	658	O	THR	A	421	45.157	54.632	9.000	1.00	77.93
	659	CB	THR	A	421	43.671	52.283	9.225	1.00	73.75
	660	OG1	THR	A	421	42.628	51.328	9.451	1.00	77.71
	661	CG2	THR	A	421	45.009	51.567	9.227	1.00	75.35
	662	N	HIS	A	422	45.499	54.624	11.226	1.00	81.02
	663	CA	HIS	A	422	46.678	55.483	11.151	1.00	86.07
	664	C	HIS	A	422	47.914	54.596	11.278	1.00	89.67
	665	O	HIS	A	422	47.947	53.680	12.098	1.00	90.00

	666	CB	HIS	A	422	46.660	56.529	12.269	1.00	87.43
	667	CG	HIS	A	422	47.548	57.708	12.008	1.00	90.73
	668	ND1	HIS	A	422	47.397	58.524	10.909	1.00	93.83
	669	CD2	HIS	A	422	48.600	58.204	12.704	1.00	91.89
	670	CE1	HIS	A	422	48.318	59.473	10.936	1.00	94.70
	671	NE2	HIS	A	422	49.060	59.300	12.015	1.00	93.25
	672	N	PRO	A	423	48.954	54.871	10.474	1.00	92.64
	673	CA	PRO	A	423	50.209	54.111	10.460	1.00	95.19
	674	C	PRO	A	423	50.838	53.628	11.775	1.00	97.06
	675	O	PRO	A	423	51.064	52.431	11.945	1.00	97.57
	676	CB	PRO	A	423	51.155	55.024	9.667	1.00	95.56
	677	CG	PRO	A	423	50.566	56.391	9.853	1.00	93.94
	678	CD	PRO	A	423	49.105	56.112	9.696	1.00	93.12
	679	N	HIS	A	424	51.105	54.542	12.701	1.00	98.71
	680	CA	HIS	A	424	51.769	54.190	13.957	1.00	100.16
	681	C	HIS	A	424	51.021	53.496	15.095	1.00	99.67
	682	O	HIS	A	424	51.609	52.690	15.816	1.00	99.61
	683	CB	HIS	A	424	52.451	55.435	14.522	1.00	102.42
	684	CG	HIS	A	424	53.475	56.022	13.605	1.00	105.47
	685	ND1	HIS	A	424	53.372	57.298	13.092	1.00	107.10
	686	CD2	HIS	A	424	54.639	55.521	13.133	1.00	97.46
	687	CE1	HIS	A	424	54.430	57.556	12.345	1.00	106.81
	688	NE2	HIS	A	424	55.215	56.494	12.353	1.00	106.61
	689	N	LEU	A	425	49.742	53.798	15.267	1.00	99.19
	690	CA	LEU	A	425	48.972	53.216	16.363	1.00	99.01
	691	C	LEU	A	425	48.692	51.714	16.284	1.00	98.36
	692	O	LEU	A	425	48.479	51.160	15.204	1.00	98.39
	693	CB	LEU	A	425	47.671	53.994	16.507	1.00	100.66
	694	CG	LEU	A	425	47.969	55.495	16.467	1.00	101.95
	695	CD1	LEU	A	425	46.683	56.285	16.569	1.00	102.59
	696	CD2	LEU	A	425	48.923	55.856	17.598	1.00	103.85
	697	N	PRO	A	426	48.685	51.038	17.448	1.00	97.57
	698	CA	PRO	A	426	48.435	49.596	17.540	1.00	96.82
	699	C	PRO	A	426	47.075	49.186	16.992	1.00	95.53
	700	O	PRO	A	426	46.990	48.560	15.937	1.00	95.77
	701	CB	PRO	A	426	48.570	49.318	19.037	1.00	97.13
	702	CG	PRO	A	426	48.106	50.605	19.660	1.00	97.88
	703	CD	PRO	A	426	48.802	51.631	18.793	1.00	97.70
	704	N	ARG	A	427	46.015	49.536	17.713	1.00	94.16
	705	CA	ARG	A	427	44.669	49.198	17.274	1.00	92.52
	706	C	ARG	A	427	44.091	50.315	16.408	1.00	89.85
	707	O	ARG	A	427	44.487	51.477	16.517	1.00	89.26
	708	CB	ARG	A	427	43.749	48.948	18.478	1.00	97.34
	709	CG	ARG	A	427	42.381	48.398	18.077	1.00	99.32
	710	CD	ARG	A	427	41.428	48.193	19.253	1.00	105.99
	711	NE	ARG	A	427	40.197	47.532	18.815	1.00	111.10
	712	CZ	ARG	A	427	39.140	47.298	19.588	1.00	111.66
	713	NH1	ARG	A	427	39.143	47.673	20.861	1.00	111.70
	714	NH2	ARG	A	427	38.078	46.679	19.087	1.00	110.09
	715	N	ALA	A	428	43.158	49.949	15.538	1.00	86.56
	716	CA	ALA	A	428	42.513	50.910	14.661	1.00	82.70
	717	C	ALA	A	428	41.389	51.602	15.423	1.00	80.03
	718	O	ALA	A	428	40.711	50.981	16.239	1.00	80.29
	719	CB	ALA	A	428	41.953	50.200	13.437	1.00	83.85
	720	N	LEU	A	429	41.203	52.892	15.164	1.00	76.76
	721	CA	LEU	A	429	40.144	53.651	15.815	1.00	72.72
	722	C	LEU	A	429	38.820	53.289	15.164	1.00	69.67
	723	O	LEU	A	429	38.742	53.128	13.947	1.00	68.64
	724	CB	LEU	A	429	40.392	55.156	15.671	1.00	73.60
	725	CG	LEU	A	429	41.169	55.847	16.793	1.00	73.35
	726	CD1	LEU	A	429	41.498	57.280	16.404	1.00	72.09
	727	CD2	LEU	A	429	40.333	55.813	18.065	1.00	76.40

	728	N	MET	A	430	37.779	53.153	15.976	1.00	66.83
	729	CA	MET	A	430	36.468	52.814	15.449	1.00	64.81
	730	C	MET	A	430	35.384	53.678	16.074	1.00	61.41
	731	O	MET	A	430	35.274	53.776	17.299	1.00	60.84
	732	CB	MET	A	430	36.173	51.335	15.691	1.00	68.22
	733	CG	MET	A	430	37.247	50.416	15.133	1.00	74.39
	734	SD	MET	A	430	36.886	48.679	15.387	1.00	83.18
	735	CE	MET	A	430	36.836	48.607	17.194	1.00	84.12
	736	N	ARG	A	431	34.590	54.312	15.218	1.00	57.17
	737	CA	ARG	A	431	33.506	55.172	15.674	1.00	54.04
	738	C	ARG	A	431	32.234	54.752	14.963	1.00	50.58
	739	O	ARG	A	431	32.270	54.367	13.796	1.00	50.46
	740	CB	ARG	A	431	33.825	56.641	15.364	1.00	55.16
	741	CG	ARG	A	431	35.036	57.187	16.109	1.00	59.24
	742	CD	ARG	A	431	34.802	57.172	17.611	1.00	63.93
	743	NE	ARG	A	431	35.983	57.586	18.363	1.00	70.30
	744	CZ	ARG	A	431	36.070	57.557	19.689	1.00	76.24
	745	NH1	ARG	A	431	35.041	57.131	20.417	1.00	77.83
	746	NH2	ARG	A	431	37.185	57.952	20.289	1.00	77.12
	747	N	SER	A	432	31.112	54.812	15.669	1.00	46.92
	748	CA	SER	A	432	29.835	54.437	15.084	1.00	45.15
	749	C	SER	A	432	28.784	55.482	15.398	1.00	42.49
	750	O	SER	A	432	28.901	56.218	16.379	1.00	42.76
	751	CB	SER	A	432	29.394	53.068	15.610	1.00	44.31
	752	OG	SER	A	432	29.316	53.084	17.018	1.00	49.96
	753	N	THR	A	433	27.749	55.540	14.570	1.00	40.28
	754	CA	THR	A	433	26.691	56.522	14.763	1.00	39.71
	755	C	THR	A	433	25.356	55.996	14.257	1.00	39.49
	756	O	THR	A	433	25.315	55.186	13.334	1.00	40.22
	757	CB	THR	A	433	27.023	57.839	14.022	1.00	38.07
	758	OG1	THR	A	433	26.006	58.807	14.295	1.00	39.56
	759	CG2	THR	A	433	27.088	57.609	12.518	1.00	36.99
	760	N	THR	A	434	24.272	56.461	14.874	1.00	39.18
	761	CA	THR	A	434	22.913	56.068	14.512	1.00	40.70
	762	C	THR	A	434	21.965	57.186	14.934	1.00	40.23
	763	O	THR	A	434	22.364	58.091	15.659	1.00	41.18
	764	CB	THR	A	434	22.484	54.784	15.256	1.00	43.01
	765	OG1	THR	A	434	22.362	55.052	16.661	1.00	47.85
	766	CG2	THR	A	434	23.524	53.726	15.105	1.00	48.67
	767	N	LYS	A	435	20.714	57.125	14.496	1.00	40.97
	768	CA	LYS	A	435	19.767	58.150	14.889	1.00	45.73
	769	C	LYS	A	435	19.601	58.021	16.398	1.00	48.93
	770	O	LYS	A	435	19.710	56.930	16.942	1.00	48.49
	771	CB	LYS	A	435	18.434	57.937	14.194	1.00	45.94
	772	N	THR	A	436	19.365	59.133	17.082	1.00	52.01
	773	CA	THR	A	436	19.171	59.080	18.526	1.00	54.88
	774	C	THR	A	436	17.722	58.684	18.774	1.00	55.70
	775	O	THR	A	436	16.823	59.146	18.077	1.00	55.21
	776	CB	THR	A	436	19.438	60.454	19.191	1.00	56.24
	777	OG1	THR	A	436	20.821	60.802	19.038	1.00	60.56
	778	CG2	THR	A	436	19.090	60.412	20.677	1.00	57.04
	779	N	SER	A	437	17.501	57.810	19.748	1.00	57.93
	780	CA	SER	A	437	16.149	57.380	20.080	1.00	60.42
	781	C	SER	A	437	15.683	58.239	21.249	1.00	60.49
	782	O	SER	A	437	16.357	59.203	21.623	1.00	60.21
	783	CB	SER	A	437	16.133	55.894	20.470	1.00	61.57
	784	OG	SER	A	437	16.957	55.651	21.600	1.00	65.51
	785	N	GLY	A	438	14.533	57.895	21.821	1.00	60.09
	786	CA	GLY	A	438	14.022	58.666	22.939	1.00	58.42
	787	C	GLY	A	438	12.937	59.630	22.511	1.00	57.80
	788	O	GLY	A	438	12.648	59.747	21.322	1.00	56.51
	789	N	PRO	A	439	12.309	60.333	23.467	1.00	57.81

	790	CA	PRO	A	439	11.242	61.295	23.185	1.00	56.19
	791	C	PRO	A	439	11.692	62.422	22.263	1.00	53.91
	792	O	PRO	A	439	12.886	62.709	22.147	1.00	53.91
	793	CB	PRO	A	439	10.865	61.806	24.576	1.00	57.79
	794	CG	PRO	A	439	11.147	60.633	25.448	1.00	58.60
	795	CD	PRO	A	439	12.485	60.173	24.921	1.00	60.65
	796	N	ARG	A	440	10.722	63.055	21.612	1.00	51.09
	797	CA	ARG	A	440	10.990	64.163	20.702	1.00	48.90
	798	C	ARG	A	440	10.220	65.365	21.231	1.00	45.83
	799	O	ARG	A	440	9.188	65.202	21.881	1.00	45.88
	800	CB	ARG	A	440	10.501	63.836	19.289	1.00	49.95
	801	CG	ARG	A	440	10.919	62.473	18.771	1.00	59.03
	802	CD	ARG	A	440	12.406	62.373	18.448	1.00	65.31
	803	NE	ARG	A	440	12.814	60.973	18.342	1.00	72.31
	804	CZ	ARG	A	440	13.986	60.553	17.878	1.00	74.99
	805	NH1	ARG	A	440	14.894	61.419	17.460	1.00	77.22
	806	NH2	ARG	A	440	14.252	59.255	17.837	1.00	78.59
	807	N	ALA	A	441	10.727	66.564	20.957	1.00	42.09
	808	CA	ALA	A	441	10.079	67.800	21.387	1.00	39.26
	809	C	ALA	A	441	10.476	68.894	20.413	1.00	38.22
	810	O	ALA	A	441	11.649	69.034	20.076	1.00	38.95
	811	CB	ALA	A	441	10.511	68.170	22.798	1.00	36.56
	812	N	ALA	A	442	9.496	69.666	19.966	1.00	37.22
	813	CA	ALA	A	442	9.739	70.729	19.011	1.00	37.60
	814	C	ALA	A	442	10.550	71.879	19.590	1.00	38.65
	815	O	ALA	A	442	10.553	72.103	20.798	1.00	40.22
	816	CB	ALA	A	442	8.415	71.248	18.481	1.00	37.17
	817	N	PRO	A	443	11.260	72.619	18.722	1.00	38.04
	818	CA	PRO	A	443	12.089	73.765	19.104	1.00	36.79
	819	C	PRO	A	443	11.224	75.019	19.243	1.00	38.14
	820	O	PRO	A	443	10.236	75.174	18.521	1.00	37.39
	821	CB	PRO	A	443	13.050	73.923	17.921	1.00	36.30
	822	CG	PRO	A	443	12.946	72.632	17.159	1.00	36.35
	823	CD	PRO	A	443	11.512	72.249	17.320	1.00	37.85
	824	N	GLU	A	444	11.594	75.894	20.173	1.00	36.28
	825	CA	GLU	A	444	10.901	77.163	20.371	1.00	35.57
	826	C	GLU	A	444	11.941	78.171	19.888	1.00	33.87
	827	O	GLU	A	444	13.110	78.105	20.291	1.00	33.43
	828	CB	GLU	A	444	10.580	77.383	21.851	1.00	38.68
	829	N	VAL	A	445	11.520	79.097	19.033	1.00	30.18
	830	CA	VAL	A	445	12.432	80.070	18.450	1.00	28.24
	831	C	VAL	A	445	12.136	81.523	18.811	1.00	28.44
	832	O	VAL	A	445	11.000	81.975	18.721	1.00	26.78
	833	CB	VAL	A	445	12.417	79.937	16.905	1.00	28.10
	834	CG1	VAL	A	445	13.370	80.933	16.274	1.00	25.56
	835	CG2	VAL	A	445	12.771	78.521	16.511	1.00	26.30
	836	N	TYR	A	446	13.175	82.251	19.203	1.00	27.87
	837	CA	TYR	A	446	13.019	83.651	19.551	1.00	27.91
	838	C	TYR	A	446	14.193	84.460	19.024	1.00	27.06
	839	O	TYR	A	446	15.326	84.307	19.480	1.00	27.96
	840	CB	TYR	A	446	12.898	83.836	21.074	1.00	26.45
	841	CG	TYR	A	446	12.749	85.289	21.447	1.00	26.59
	842	CD1	TYR	A	446	11.714	86.057	20.905	1.00	28.48
	843	CD2	TYR	A	446	13.659	85.914	22.305	1.00	29.02
	844	CE1	TYR	A	446	11.589	87.417	21.204	1.00	33.24
	845	CE2	TYR	A	446	13.543	87.274	22.616	1.00	31.33
	846	CZ	TYR	A	446	12.506	88.015	22.059	1.00	36.01
	847	OH	TYR	A	446	12.387	89.352	22.338	1.00	36.54
	848	N	ALA	A	447	13.914	85.326	18.060	1.00	28.07
	849	CA	ALA	A	447	14.949	86.150	17.439	1.00	27.67
	850	C	ALA	A	447	14.815	87.579	17.932	1.00	29.19
	851	O	ALA	A	447	13.702	88.036	18.173	1.00	31.10

	852	CB	ALA	A	447	14.802	86.098	15.931	1.00	23.97
	853	N	PHE	A	448	15.929	88.293	18.079	1.00	29.56
	854	CA	PHE	A	448	15.849	89.657	18.578	1.00	32.50
	855	C	PHE	A	448	17.075	90.483	18.246	1.00	33.67
	856	O	PHE	A	448	18.112	89.950	17.872	1.00	35.26
	857	CB	PHE	A	448	15.659	89.630	20.097	1.00	35.29
	858	CG	PHE	A	448	16.849	89.077	20.838	1.00	37.04
	859	CD1	PHE	A	448	17.912	89.909	21.295	1.00	36.66
	860	CD2	PHE	A	448	16.934	87.714	21.127	1.00	34.95
	861	CE1	PHE	A	448	19.049	89.382	21.824	1.00	40.91
	862	CE2	PHE	A	448	18.066	87.178	21.753	1.00	35.99
	863	CZ	PHE	A	448	19.123	88.014	22.103	1.00	35.15
	864	N	ALA	A	449	16.952	91.796	18.396	1.00	35.81
	865	CA	ALA	A	449	18.066	92.693	18.131	1.00	37.63
	866	C	ALA	A	449	18.617	93.253	19.438	1.00	40.96
	867	O	ALA	A	449	17.885	93.441	20.403	1.00	40.14
	868	CB	ALA	A	449	17.623	93.831	17.230	1.00	33.60
	869	N	THR	A	450	19.918	93.509	19.448	1.00	45.40
	870	CA	THR	A	450	20.606	94.071	20.595	1.00	50.82
	871	C	THR	A	450	20.515	95.597	20.498	1.00	53.78
	872	O	THR	A	450	20.673	96.169	19.417	1.00	54.14
	873	CB	THR	A	450	22.090	93.665	20.587	1.00	51.45
	874	OG1	THR	A	450	22.192	92.242	20.450	1.00	54.12
	875	CG2	THR	A	450	22.769	94.093	21.877	1.00	55.58
	876	N	PRO	A	451	20.260	96.275	21.626	1.00	56.74
	877	CA	PRO	A	451	20.157	97.737	21.623	1.00	59.05
	878	C	PRO	A	451	21.427	98.391	21.080	1.00	61.00
	879	O	PRO	A	451	22.535	98.080	21.521	1.00	59.71
	880	CB	PRO	A	451	19.933	98.073	23.098	1.00	60.52
	881	CG	PRO	A	451	19.262	96.851	23.640	1.00	61.14
	882	CD	PRO	A	451	20.049	95.739	22.981	1.00	59.39
	883	N	GLU	A	452	21.272	99.285	20.112	1.00	64.30
	884	CA	GLU	A	452	22.428	99.975	19.558	1.00	69.17
	885	C	GLU	A	452	22.252	101.463	19.842	1.00	72.61
	886	O	GLU	A	452	21.667	102.206	19.057	1.00	73.59
	887	CB	GLU	A	452	22.560	99.712	18.054	1.00	65.66
	888	CG	GLU	A	452	24.015	99.566	17.577	1.00	61.46
	889	CD	GLU	A	452	24.717	98.317	18.133	1.00	60.52
	890	OE1	GLU	A	452	24.053	97.264	18.251	1.00	63.47
	891	OE2	GLU	A	452	25.934	98.373	18.433	1.00	53.34
	892	N	TRP	A	453	22.763	101.869	20.997	1.00	76.75
	893	CA	TRP	A	453	22.693	103.242	21.481	1.00	81.00
	894	C	TRP	A	453	23.886	104.027	20.913	1.00	82.30
	895	O	TRP	A	453	25.038	103.710	21.215	1.00	82.08
	896	CB	TRP	A	453	22.737	103.191	23.010	1.00	85.65
	897	CG	TRP	A	453	22.182	104.367	23.734	1.00	89.76
	898	CD1	TRP	A	453	20.939	104.921	23.588	1.00	92.34
	899	CD2	TRP	A	453	22.819	105.083	24.795	1.00	94.15
	900	NE1	TRP	A	453	20.764	105.934	24.502	1.00	94.99
	901	CE2	TRP	A	453	21.904	106.055	25.255	1.00	95.56
	902	CE3	TRP	A	453	24.079	104.995	25.407	1.00	95.36
	903	CZ2	TRP	A	453	22.208	106.935	26.300	1.00	97.14
	904	CZ3	TRP	A	453	24.380	105.869	26.445	1.00	95.61
	905	CH2	TRP	A	453	23.447	106.826	26.880	1.00	97.12
	906	N	PRO	A	454	23.619	105.058	20.080	1.00	84.10
	907	CA	PRO	A	454	24.606	105.931	19.422	1.00	87.24
	908	C	PRO	A	454	25.892	106.316	20.162	1.00	90.52
	909	O	PRO	A	454	26.088	105.978	21.333	1.00	89.75
	910	CB	PRO	A	454	23.775	107.150	18.988	1.00	84.91
	911	CG	PRO	A	454	22.475	107.017	19.740	1.00	83.62
	912	CD	PRO	A	454	22.259	105.537	19.793	1.00	84.60
	913	N	GLY	A	455	26.751	107.055	19.464	1.00	91.72

	914	CA	GLY	A	455	28.048	107.413	20.012	1.00	94.13
	915	C	GLY	A	455	28.730	106.132	19.601	1.00	96.28
	916	O	GLY	A	455	28.613	105.125	20.301	1.00	97.74
40	917	N	SER	A	456	29.442	106.142	18.478	1.00	99.11
	918	CA	SER	A	456	29.974	104.869	18.023	1.00	96.15
	919	C	SER	A	456	31.407	104.465	17.676	1.00	91.50
	920	O	SER	A	456	32.292	105.284	17.333	1.00	88.52
	921	CB	SER	A	456	29.092	104.378	16.879	1.00	95.05
45	922	OG	SER	A	456	28.910	105.375	15.884	1.00	110.76
	923	N	ARG	A	457	31.541	103.136	17.752	1.00	87.73
	924	CA	ARG	A	457	32.664	102.251	17.520	1.00	87.81
	925	C	ARG	A	457	31.678	101.103	17.647	1.00	86.30
	926	O	ARG	A	457	31.026	100.998	18.697	1.00	90.57
50	927	CB	ARG	A	457	33.634	102.261	18.675	1.00	94.67
	928	N	ASP	A	458	31.512	100.259	16.627	1.00	87.32
	929	CA	ASP	A	458	30.441	99.286	16.780	1.00	80.43
	930	C	ASP	A	458	30.422	97.963	16.080	1.00	72.83
	931	O	ASP	A	458	31.410	97.437	15.599	1.00	73.96
55	932	CB	ASP	A	458	29.150	99.985	16.385	1.00	83.19
	933	CG	ASP	A	458	29.102	100.300	14.890	1.00	85.09
	934	OD1	ASP	A	458	30.065	100.906	14.378	1.00	91.25
	935	OD2	ASP	A	458	28.108	99.939	14.217	1.00	90.84
	936	N	LYS	A	459	29.196	97.451	16.076	1.00	66.05
5	937	CA	LYS	A	459	28.782	96.211	15.437	1.00	61.75
	938	C	LYS	A	459	27.368	95.983	15.886	1.00	56.14
	939	O	LYS	A	459	27.144	95.648	17.046	1.00	56.54
	940	CB	LYS	A	459	29.641	95.031	15.889	1.00	68.18
	941	CG	LYS	A	459	30.801	94.804	14.969	1.00	71.85
10	942	CD	LYS	A	459	30.406	94.863	13.499	1.00	73.79
	943	CE	LYS	A	459	31.655	94.839	12.626	1.00	76.14
	944	NZ	LYS	A	459	31.341	94.675	11.169	1.00	79.35
	945	N	ARG	A	460	26.406	96.194	15.001	1.00	52.32
	946	CA	ARG	A	460	25.035	95.951	15.377	1.00	47.59
15	947	C	ARG	A	460	24.860	94.436	15.290	1.00	43.34
	948	O	ARG	A	460	25.477	93.761	14.462	1.00	40.40
	949	CB	ARG	A	460	24.104	96.726	14.456	1.00	49.27
	950	CG	ARG	A	460	24.275	98.216	14.671	1.00	56.23
	951	CD	ARG	A	460	23.659	99.006	13.532	1.00	63.20
20	952	NE	ARG	A	460	23.997	100.426	13.596	1.00	68.02
	953	CZ	ARG	A	460	25.145	100.955	13.180	1.00	70.46
	954	NH1	ARG	A	460	26.094	100.185	12.656	1.00	72.23
	955	NH2	ARG	A	460	25.336	102.264	13.285	1.00	73.53
	956	N	THR	A	461	24.062	93.910	16.198	1.00	39.19
25	957	CA	THR	A	461	23.879	92.474	16.278	1.00	36.81
	958	C	THR	A	461	22.447	92.004	16.401	1.00	34.03
	959	O	THR	A	461	21.631	92.607	17.110	1.00	33.96
	960	CB	THR	A	461	24.603	91.890	17.512	1.00	39.13
	961	OG1	THR	A	461	25.957	92.357	17.557	1.00	46.04
30	962	CG2	THR	A	461	24.630	90.380	17.421	1.00	45.48
	963	N	LEU	A	462	22.157	90.904	15.714	1.00	29.84
	964	CA	LEU	A	462	20.853	90.267	15.788	1.00	28.03
	965	C	LEU	A	462	21.205	88.926	16.410	1.00	27.33
	966	O	LEU	A	462	22.307	88.414	16.207	1.00	24.47
35	967	CB	LEU	A	462	20.223	90.074	14.403	1.00	25.97
	968	CG	LEU	A	462	19.888	91.362	13.635	1.00	33.39
	969	CD1	LEU	A	462	19.172	91.007	12.319	1.00	32.36
	970	CD2	LEU	A	462	19.014	92.263	14.483	1.00	30.72
	971	N	ALA	A	463	20.286	88.359	17.178	1.00	25.83
40	972	CA	ALA	A	463	20.577	87.111	17.836	1.00	25.65
	973	C	ALA	A	463	19.330	86.279	17.957	1.00	26.32
	974	O	ALA	A	463	18.214	86.790	17.846	1.00	27.53
	975	CB	ALA	A	463	21.179	87.381	19.212	1.00	28.15

	976	N	CYS	A	464	19.518	84.992	18.195	1.00	21.23
	977	CA	CYS	A	464	18.388	84.093	18.276	1.00	24.77
	978	C	CYS	A	464	18.599	83.016	19.314	1.00	22.14
	979	O	CYS	A	464	19.683	82.431	19.402	1.00	24.66
	980	CB	CYS	A	464	18.193	83.429	16.914	1.00	22.04
	981	SG	CYS	A	464	16.790	82.298	16.720	1.00	34.06
	982	N	LEU	A	465	17.548	82.741	20.075	1.00	22.44
	983	CA	LEU	A	465	17.598	81.697	21.089	1.00	23.11
	984	C	LEU	A	465	16.644	80.615	20.641	1.00	22.43
	985	O	LEU	A	465	15.483	80.898	20.352	1.00	23.73
	986	CB	LEU	A	465	17.155	82.230	22.461	1.00	22.99
	987	CG	LEU	A	465	16.810	81.177	23.538	1.00	19.04
	988	CD1	LEU	A	465	18.035	80.331	23.866	1.00	21.72
	989	CD2	LEU	A	465	16.347	81.884	24.818	1.00	28.23
	990	N	ILE	A	466	17.125	79.380	20.581	1.00	22.56
	991	CA	ILE	A	466	16.277	78.268	20.169	1.00	22.11
	992	C	ILE	A	466	16.302	77.256	21.297	1.00	24.25
	993	O	ILE	A	466	17.375	76.815	21.706	1.00	24.93
	994	CB	ILE	A	466	16.781	77.654	18.861	1.00	22.15
	995	CG1	ILE	A	466	16.849	78.750	17.786	1.00	23.07
	996	CG2	ILE	A	466	15.822	76.525	18.416	1.00	25.24
	997	CD1	ILE	A	466	17.509	78.318	16.496	1.00	33.12
	998	N	GLN	A	467	15.132	76.863	21.793	1.00	24.63
	999	CA	GLN	A	467	15.120	75.970	22.951	1.00	28.64
	1000	C	GLN	A	467	13.982	74.963	23.072	1.00	31.08
	1001	O	GLN	A	467	13.071	74.915	22.235	1.00	31.00
	1002	CB	GLN	A	467	15.172	76.830	24.228	1.00	25.58
	1003	CG	GLN	A	467	13.943	77.727	24.404	1.00	25.53
	1004	CD	GLN	A	467	14.044	78.693	25.599	1.00	30.72
	1005	OE1	GLN	A	467	14.790	78.456	26.549	1.00	29.76
	1006	NE2	GLN	A	467	13.273	79.779	25.550	1.00	32.18
	1007	N	ASN	A	468	14.083	74.147	24.123	1.00	33.71
	1008	CA	ASN	A	468	13.114	73.106	24.459	1.00	36.96
	1009	C	ASN	A	468	12.993	71.999	23.423	1.00	38.20
	1010	O	ASN	A	468	11.931	71.392	23.288	1.00	38.39
	1011	CB	ASN	A	468	11.731	73.719	24.676	1.00	41.06
	1012	CG	ASN	A	468	11.748	74.837	25.686	1.00	46.41
	1013	OD1	ASN	A	468	12.372	74.721	26.741	1.00	50.82
	1014	ND2	ASN	A	468	11.052	75.928	25.376	1.00	53.31
	1015	N	PHE	A	469	14.065	71.732	22.685	1.00	35.74
	1016	CA	PHE	A	469	14.003	70.690	21.677	1.00	33.87
	1017	C	PHE	A	469	14.804	69.453	22.056	1.00	33.63
	1018	O	PHE	A	469	15.727	69.513	22.860	1.00	34.78
	1019	CB	PHE	A	469	14.495	71.228	20.322	1.00	29.12
	1020	CG	PHE	A	469	15.926	71.691	20.334	1.00	26.27
	1021	CD1	PHE	A	469	16.959	70.792	20.133	1.00	22.45
	1022	CD2	PHE	A	469	16.238	73.034	20.539	1.00	22.06
	1023	CE1	PHE	A	469	18.285	71.214	20.126	1.00	23.84
	1024	CE2	PHE	A	469	17.564	73.465	20.536	1.00	28.02
	1025	CZ	PHE	A	469	18.593	72.549	20.327	1.00	23.33
	1026	N	MET	A	470	14.431	68.327	21.466	1.00	35.64
	1027	CA	MET	A	470	15.120	67.065	21.687	1.00	37.62
	1028	C	MET	A	470	14.684	66.104	20.596	1.00	36.36
	1029	O	MET	A	470	13.529	66.122	20.177	1.00	36.33
	1030	CB	MET	A	470	14.804	66.495	23.076	1.00	42.61
	1031	CG	MET	A	470	13.354	66.179	23.350	1.00	50.60
	1032	SD	MET	A	470	13.141	65.744	25.113	1.00	66.08
	1033	CE	MET	A	470	13.780	64.056	25.134	1.00	66.35
	1034	N	PRO	A	471	15.613	65.283	20.079	1.00	34.63
	1035	CA	PRO	A	471	17.039	65.169	20.418	1.00	32.61
	1036	C	PRO	A	471	17.818	66.453	20.143	1.00	31.92
	1037	O	PRO	A	471	17.244	67.436	19.685	1.00	29.59

	1038	CB	PRO	A	471	17.520	64.015	19.538	1.00	33.95
	1039	CG	PRO	A	471	16.277	63.227	19.295	1.00	37.90
	1040	CD	PRO	A	471	15.246	64.291	19.058	1.00	34.78
	1041	N	GLU	A	472	19.128	66.413	20.386	1.00	32.28
	1042	CA	GLU	A	472	20.001	67.580	20.234	1.00	36.49
	1043	C	GLU	A	472	20.380	68.043	18.830	1.00	35.52
	1044	O	GLU	A	472	20.870	69.162	18.683	1.00	34.87
	1045	CB	GLU	A	472	21.302	67.377	21.015	1.00	41.97
	1046	CG	GLU	A	472	22.213	66.306	20.423	1.00	54.78
	1047	CD	GLU	A	472	23.527	66.144	21.184	1.00	62.41
	1048	OE1	GLU	A	472	23.603	66.579	22.356	1.00	67.26
	1049	OE2	GLU	A	472	24.481	65.566	20.613	1.00	64.96
	1050	N	ASP	A	473	20.161	67.221	17.805	1.00	34.38
	1051	CA	ASP	A	473	20.543	67.629	16.452	1.00	31.83
	1052	C	ASP	A	473	19.602	68.686	15.886	1.00	31.24
	1053	O	ASP	A	473	18.380	68.528	15.901	1.00	31.80
	1054	CB	ASP	A	473	20.621	66.420	15.516	1.00	34.73
	1055	CG	ASP	A	473	21.746	65.453	15.904	1.00	40.83
	1056	OD1	ASP	A	473	22.841	65.924	16.296	1.00	44.18
	1057	OD2	ASP	A	473	21.539	64.222	15.810	1.00	40.17
	1058	N	ILE	A	474	20.184	69.774	15.398	1.00	26.96
	1059	CA	ILE	A	474	19.393	70.856	14.854	1.00	25.39
	1060	C	ILE	A	474	20.225	71.715	13.892	1.00	24.74
	1061	O	ILE	A	474	21.436	71.824	14.031	1.00	25.20
	1062	CB	ILE	A	474	18.842	71.738	16.008	1.00	23.81
	1063	CG1	ILE	A	474	17.748	72.675	15.502	1.00	22.23
	1064	CG2	ILE	A	474	19.974	72.538	16.647	1.00	27.10
	1065	CD1	ILE	A	474	17.064	73.456	16.650	1.00	25.30
	1066	N	SER	A	475	19.570	72.288	12.891	1.00	23.27
	1067	CA	SER	A	475	20.252	73.170	11.952	1.00	22.17
	1068	C	SER	A	475	19.609	74.534	12.148	1.00	21.71
	1069	O	SER	A	475	18.393	74.649	12.224	1.00	20.84
	1070	CB	SER	A	475	20.049	72.721	10.507	1.00	20.43
	1071	OG	SER	A	475	20.589	71.436	10.294	1.00	30.00
	1072	N	VAL	A	476	20.442	75.558	12.213	1.00	21.76
	1073	CA	VAL	A	476	19.980	76.906	12.425	1.00	21.72
	1074	C	VAL	A	476	20.435	77.725	11.249	1.00	23.56
	1075	O	VAL	A	476	21.555	77.564	10.780	1.00	25.95
	1076	CB	VAL	A	476	20.606	77.513	13.715	1.00	21.56
	1077	CG1	VAL	A	476	20.157	78.975	13.878	1.00	18.70
	1078	CG2	VAL	A	476	20.197	76.685	14.934	1.00	20.99
	1079	N	GLN	A	477	19.574	78.606	10.764	1.00	25.16
	1080	CA	GLN	A	477	19.965	79.428	9.640	1.00	26.65
	1081	C	GLN	A	477	19.263	80.767	9.662	1.00	26.62
	1082	O	GLN	A	477	18.160	80.891	10.175	1.00	26.40
	1083	CB	GLN	A	477	19.701	78.683	8.325	1.00	31.51
	1084	CG	GLN	A	477	18.289	78.252	8.089	1.00	44.27
	1085	CD	GLN	A	477	18.188	77.095	7.084	1.00	47.76
	1086	OE1	GLN	A	477	17.104	76.786	6.598	1.00	50.57
	1087	NE2	GLN	A	477	19.317	76.449	6.787	1.00	47.32
	1088	N	TRP	A	478	19.941	81.780	9.146	1.00	27.41
	1089	CA	TRP	A	478	19.375	83.112	9.074	1.00	28.36
	1090	C	TRP	A	478	18.944	83.408	7.635	1.00	30.10
	1091	O	TRP	A	478	19.567	82.940	6.672	1.00	25.31
	1092	CB	TRP	A	478	20.404	84.139	9.533	1.00	28.76
	1093	CG	TRP	A	478	20.649	84.098	11.013	1.00	34.11
	1094	CD1	TRP	A	478	21.522	83.287	11.685	1.00	31.25
	1095	CD2	TRP	A	478	19.980	84.878	12.006	1.00	31.01
	1096	NE1	TRP	A	478	21.436	83.515	13.031	1.00	27.71
	1097	CE2	TRP	A	478	20.496	84.487	13.259	1.00	31.95

	1098	CE3	TRP	A	478	18.993	85.871	11.960	1.00	34.16
	1099	CZ2	TRP	A	478	20.055	85.058	14.463	1.00	25.26
	1100	CZ3	TRP	A	478	18.556	86.439	13.153	1.00	31.64
	1101	CH2	TRP	A	478	19.089	86.029	14.387	1.00	28.89
	1102	N	LEU	A	479	17.877	84.182	7.498	1.00	32.48
	1103	CA	LEU	A	479	17.355	84.551	6.187	1.00	37.36
	1104	C	LEU	A	479	16.943	86.016	6.140	1.00	40.42
	1105	O	LEU	A	479	16.448	86.560	7.123	1.00	40.14
	1106	CB	LEU	A	479	16.122	83.722	5.848	1.00	39.83
	1107	CG	LEU	A	479	16.044	82.254	6.258	1.00	44.57
	1108	CD1	LEU	A	479	14.713	81.710	5.810	1.00	52.98
	1109	CD2	LEU	A	479	17.161	81.470	5.634	1.00	50.71
	1110	N	HIS	A	480	17.152	86.653	4.998	1.00	43.05
	1111	CA	HIS	A	480	16.723	88.028	4.824	1.00	49.20
	1112	C	HIS	A	480	15.464	87.854	3.984	1.00	52.73
	1113	O	HIS	A	480	15.509	87.895	2.753	1.00	52.90
	1114	CB	HIS	A	480	17.756	88.846	4.057	1.00	52.25
	1115	CG	HIS	A	480	17.330	90.259	3.814	1.00	57.22
	1116	ND1	HIS	A	480	17.525	91.263	4.736	1.00	61.37
	1117	CD2	HIS	A	480	16.658	90.822	2.781	1.00	59.16
	1118	CE1	HIS	A	480	16.993	92.384	4.285	1.00	59.88
	1119	NE2	HIS	A	480	16.460	92.144	3.100	1.00	66.11
	1120	N	ASN	A	481	14.347	87.629	4.670	1.00	56.65
	1121	CA	ASN	A	481	13.057	87.394	4.030	1.00	59.93
	1122	C	ASN	A	481	13.009	85.940	3.581	1.00	59.65
	1123	O	ASN	A	481	13.031	85.029	4.405	1.00	61.04
	1124	CB	ASN	A	481	12.849	88.312	2.818	1.00	64.65
	1125	CG	ASN	A	481	12.578	89.748	3.210	1.00	72.38
	1126	OD1	ASN	A	481	11.636	90.037	3.953	1.00	74.96
	1127	ND2	ASN	A	481	13.401	90.662	2.707	1.00	75.60
	1128	N	GLU	A	482	12.975	85.728	2.273	1.00	58.97
	1129	CA	GLU	A	482	12.903	84.387	1.704	1.00	58.55
	1130	C	GLU	A	482	14.254	83.785	1.318	1.00	55.30
	1131	O	GLU	A	482	14.347	82.587	1.056	1.00	57.27
	1132	CB	GLU	A	482	11.993	84.424	0.473	1.00	65.42
	1133	CG	GLU	A	482	11.787	85.840	-0.072	1.00	73.94
	1134	CD	GLU	A	482	11.127	85.865	-1.432	1.00	80.29
	1135	OE1	GLU	A	482	11.770	85.432	-2.413	1.00	86.31
	1136	OE2	GLU	A	482	9.967	86.316	-1.520	1.00	82.73
	1137	N	VAL	A	483	15.299	84.603	1.286	1.00	50.25
	1138	CA	VAL	A	483	16.612	84.113	0.889	1.00	45.78
	1139	C	VAL	A	483	17.575	83.867	2.048	1.00	43.04
	1140	O	VAL	A	483	17.766	84.720	2.902	1.00	41.34
	1141	CB	VAL	A	483	17.261	85.073	-0.133	1.00	43.76
	1142	CG1	VAL	A	483	17.317	86.471	0.432	1.00	46.25
	1143	CG2	VAL	A	483	18.654	84.589	-0.494	1.00	41.37
	1144	N	GLN	A	484	18.188	82.688	2.050	1.00	42.30
	1145	CA	GLN	A	484	19.126	82.300	3.095	1.00	43.21
	1146	C	GLN	A	484	20.509	82.942	2.959	1.00	42.48
	1147	O	GLN	A	484	21.055	83.062	1.856	1.00	41.64
	1148	CB	GLN	A	484	19.269	80.774	3.129	1.00	45.96
	1149	CG	GLN	A	484	20.331	80.276	4.101	1.00	54.43
	1150	CD	GLN	A	484	20.427	78.760	4.159	1.00	59.02
	1151	OE1	GLN	A	484	21.400	78.209	4.677	1.00	59.71
	1152	NE2	GLN	A	484	19.410	78.078	3.636	1.00	61.46
	1153	N	LEU	A	485	21.061	83.361	4.094	1.00	38.99
	1154	CA	LEU	A	485	22.382	83.982	4.147	1.00	39.17
	1155	C	LEU	A	485	23.458	82.900	4.247	1.00	40.35
	1156	O	LEU	A	485	23.183	81.778	4.670	1.00	37.39
	1157	CB	LEU	A	485	22.493	84.895	5.375	1.00	37.16

1158	CG	LEU	A	485	21.460	86.021	5.498	1.00	39.66
1159	CD1	LEU	A	485	21.670	86.764	6.807	1.00	39.30
1160	CD2	LEU	A	485	21.580	86.956	4.305	1.00	40.56
1161	N	PRO	A	486	24.700	83.227	3.858	1.00	42.55
1162	CA	PRO	A	486	25.772	82.234	3.942	1.00	46.30
1163	C	PRO	A	486	25.940	81.850	5.412	1.00	49.32
1164	O	PRO	A	486	25.748	82.684	6.294	1.00	48.81
1165	CB	PRO	A	486	26.991	82.994	3.425	1.00	45.64
1166	CG	PRO	A	486	26.413	84.068	2.572	1.00	45.29
1167	CD	PRO	A	486	25.206	84.505	3.331	1.00	40.65
1168	N	ASP	A	487	26.310	80.603	5.671	1.00	53.39
1169	CA	ASP	A	487	26.507	80.135	7.038	1.00	57.75
1170	C	ASP	A	487	27.603	80.940	7.750	1.00	57.25
1171	O	ASP	A	487	27.424	81.395	8.887	1.00	57.75
1172	CB	ASP	A	487	26.892	78.656	7.023	1.00	67.82
1173	CG	ASP	A	487	26.821	78.023	8.397	1.00	76.17
1174	OD1	ASP	A	487	27.291	78.655	9.366	1.00	84.77
1175	OD2	ASP	A	487	26.303	76.889	8.508	1.00	86.94
1176	N	ALA	A	488	28.727	81.122	7.065	1.00	54.64
1177	CA	ALA	A	488	29.871	81.848	7.607	1.00	53.45
1178	C	ALA	A	488	29.531	83.179	8.263	1.00	52.74
1179	O	ALA	A	488	30.359	83.757	8.966	1.00	53.06
1180	CB	ALA	A	488	30.892	82.070	6.515	1.00	53.75
1181	N	ARG	A	489	28.313	83.662	8.044	1.00	50.96
1182	CA	ARG	A	489	27.896	84.940	8.609	1.00	47.84
1183	C	ARG	A	489	27.436	84.895	10.064	1.00	45.10
1184	O	ARG	A	489	27.442	85.919	10.737	1.00	43.37
1185	CB	ARG	A	489	26.792	85.554	7.746	1.00	48.99
1186	CG	ARG	A	489	27.306	86.368	6.576	1.00	50.01
1187	CD	ARG	A	489	27.173	87.839	6.873	1.00	50.36
1188	NE	ARG	A	489	26.019	88.413	6.195	1.00	56.65
1189	CZ	ARG	A	489	25.434	89.552	6.543	1.00	58.23
1190	NH1	ARG	A	489	25.886	90.248	7.578	1.00	61.07
1191	NH2	ARG	A	489	24.407	90.006	5.840	1.00	59.63
1192	N	HIS	A	490	27.027	83.728	10.549	1.00	42.41
1193	CA	HIS	A	490	26.576	83.635	11.934	1.00	41.63
1194	C	HIS	A	490	27.390	82.648	12.766	1.00	39.71
1195	O	HIS	A	490	28.129	81.832	12.235	1.00	41.30
1196	CB	HIS	A	490	25.092	83.252	12.000	1.00	42.40
1197	CG	HIS	A	490	24.793	81.880	11.486	1.00	43.27
1198	ND1	HIS	A	490	24.423	81.634	10.181	1.00	42.27
1199	CD2	HIS	A	490	24.821	80.674	12.101	1.00	44.41
1200	CE1	HIS	A	490	24.236	80.338	10.014	1.00	39.88
1201	NE2	HIS	A	490	24.470	79.732	11.166	1.00	45.37
1202	N	SER	A	491	27.245	82.742	14.080	1.00	37.20
1203	CA	SER	A	491	27.946	81.866	15.005	1.00	36.36
1204	C	SER	A	491	26.915	81.199	15.927	1.00	33.06
1205	O	SER	A	491	26.172	81.879	16.639	1.00	33.77
1206	CB	SER	A	491	28.949	82.690	15.812	1.00	35.42
1207	OG	SER	A	491	29.547	81.906	16.818	1.00	43.65
1208	N	THR	A	492	26.878	79.872	15.912	1.00	29.90
1209	CA	THR	A	492	25.927	79.105	16.717	1.00	29.91
1210	C	THR	A	492	26.623	78.278	17.813	1.00	29.20
1211	O	THR	A	492	27.609	77.604	17.548	1.00	30.85
1212	CB	THR	A	492	25.094	78.153	15.802	1.00	29.85
1213	OG1	THR	A	492	24.403	78.930	14.819	1.00	35.86
1214	CG2	THR	A	492	24.059	77.366	16.602	1.00	28.05
1215	N	THR	A	493	26.095	78.319	19.035	1.00	29.49
1216	CA	THR	A	493	26.687	77.568	20.143	1.00	30.19
1217	C	THR	A	493	26.305	76.099	20.044	1.00	32.39
1218	O	THR	A	493	25.390	75.737	19.314	1.00	30.70
1219	CB	THR	A	493	26.222	78.098	21.532	1.00	27.82

	1220	OG1	THR	A	493	24.794	78.008	21.640	1.00	30.48
	1221	CG2	THR	A	493	26.647	79.533	21.728	1.00	22.03
	1222	N	GLN	A	494	27.014	75.253	20.778	1.00	35.09
	1223	CA	GLN	A	494	26.721	73.821	20.770	1.00	38.19
	1224	C	GLN	A	494	25.509	73.568	21.651	1.00	36.48
	1225	O	GLN	A	494	25.330	74.240	22.668	1.00	35.75
	1226	CB	GLN	A	494	27.904	73.019	21.325	1.00	43.09
	1227	CG	GLN	A	494	29.167	73.098	20.490	1.00	58.35
	1228	CD	GLN	A	494	28.934	72.671	19.058	1.00	65.11
	1229	OE1	GLN	A	494	28.391	71.597	18.797	1.00	71.67
	1230	NE2	GLN	A	494	29.345	73.512	18.118	1.00	71.87
	1231	N	PRO	A	495	24.661	72.598	21.272	1.00	36.89
	1232	CA	PRO	A	495	23.470	72.278	22.063	1.00	38.37
	1233	C	PRO	A	495	23.863	71.991	23.513	1.00	40.80
	1234	O	PRO	A	495	24.837	71.286	23.773	1.00	40.76
	1235	CB	PRO	A	495	22.920	71.043	21.371	1.00	37.83
	1236	CG	PRO	A	495	23.300	71.285	19.926	1.00	40.41
	1237	CD	PRO	A	495	24.716	71.791	20.039	1.00	35.81
	1238	N	ARG	A	496	23.120	72.560	24.450	1.00	42.05
	1239	CA	ARG	A	496	23.392	72.345	25.860	1.00	47.69
	1240	C	ARG	A	496	22.146	71.828	26.558	1.00	51.66
	1241	O	ARG	A	496	21.042	72.317	26.316	1.00	51.95
	1242	CB	ARG	A	496	23.849	73.646	26.516	1.00	45.81
	1243	CG	ARG	A	496	25.283	74.001	26.208	1.00	51.53
	1244	CD	ARG	A	496	25.653	75.383	26.709	1.00	53.72
	1245	NE	ARG	A	496	27.046	75.425	27.137	1.00	57.50
	1246	CZ	ARG	A	496	27.478	74.992	28.317	1.00	58.59
	1247	NH1	ARG	A	496	26.626	74.489	29.199	1.00	57.22
	1248	NH2	ARG	A	496	28.768	75.058	28.612	1.00	65.31
	1249	N	LYS	A	497	22.319	70.827	27.413	1.00	56.98
	1250	CA	LYS	A	497	21.192	70.265	28.147	1.00	61.91
	1251	C	LYS	A	497	20.733	71.299	29.145	1.00	63.97
	1252	O	LYS	A	497	21.405	72.300	29.371	1.00	64.61
	1253	CB	LYS	A	497	21.597	69.013	28.928	1.00	66.35
	1254	CG	LYS	A	497	21.819	67.752	28.113	1.00	74.14
	1255	CD	LYS	A	497	22.241	66.607	29.034	1.00	80.69
	1256	CE	LYS	A	497	22.408	65.296	28.286	1.00	84.48
	1257	NZ	LYS	A	497	22.861	64.215	29.211	1.00	88.26
	1258	N	THR	A	498	19.583	71.045	29.748	1.00	67.67
	1259	CA	THR	A	498	19.028	71.931	30.758	1.00	71.26
	1260	C	THR	A	498	18.316	71.050	31.760	1.00	73.04
	1261	O	THR	A	498	18.610	69.857	31.864	1.00	72.83
	1262	CB	THR	A	498	18.015	72.921	30.155	1.00	71.80
	1263	OG1	THR	A	498	17.045	72.208	29.379	1.00	71.58
	1264	CG2	THR	A	498	18.722	73.930	29.281	1.00	73.61
	1265	N	LYS	A	499	17.380	71.638	32.495	1.00	75.57
	1266	CA	LYS	A	499	16.607	70.895	33.480	1.00	77.62
	1267	C	LYS	A	499	15.458	70.173	32.779	1.00	77.92
	1268	O	LYS	A	499	14.504	70.809	32.332	1.00	79.19
	1269	CB	LYS	A	499	16.042	71.848	34.533	1.00	80.22
	1270	CG	LYS	A	499	17.069	72.428	35.496	1.00	81.04
	1271	CD	LYS	A	499	17.507	71.397	36.529	1.00	83.26
	1272	CE	LYS	A	499	18.368	72.031	37.613	1.00	84.81
	1273	NZ	LYS	A	499	18.736	71.055	38.675	1.00	86.04
	1274	N	GLY	A	500	15.566	68.852	32.667	1.00	76.91
	1275	CA	GLY	A	500	14.523	68.056	32.039	1.00	75.83
	1276	C	GLY	A	500	14.040	68.459	30.655	1.00	75.14
	1277	O	GLY	A	500	14.024	67.629	29.745	1.00	75.52
	1278	N	SER	A	501	13.642	69.718	30.495	1.00	73.08
	1279	CA	SER	A	501	13.132	70.230	29.225	1.00	71.65
	1280	C	SER	A	501	13.764	69.592	27.994	1.00	68.64
	1281	O	SER	A	501	13.085	68.910	27.223	1.00	71.13

	1282	CB	SER	A	501	13.321	71.746	29.147	1.00	74.43
	1283	OG	SER	A	501	14.667	72.076	28.859	1.00	80.92
	1284	N	GLY	A	502	15.060	69.814	27.810	1.00	63.14
	1285	CA	GLY	A	502	15.741	69.256	26.657	1.00	54.62
	1286	C	GLY	A	502	16.982	70.048	26.297	1.00	48.04
	1287	O	GLY	A	502	17.917	70.131	27.094	1.00	48.08
	1288	N	PHE	A	503	17.001	70.642	25.106	1.00	40.50
	1289	CA	PHE	A	503	18.173	71.411	24.692	1.00	33.81
	1290	C	PHE	A	503	17.908	72.827	24.212	1.00	28.39
	1291	O	PHE	A	503	16.789	73.192	23.856	1.00	26.35
	1292	CB	PHE	A	503	18.938	70.681	23.583	1.00	35.09
	1293	CG	PHE	A	503	19.452	69.337	23.981	1.00	34.16
	1294	CD1	PHE	A	503	18.630	68.219	23.926	1.00	35.05
	1295	CD2	PHE	A	503	20.755	69.189	24.430	1.00	35.90
	1296	CE1	PHE	A	503	19.099	66.967	24.317	1.00	36.00
	1297	CE2	PHE	A	503	21.238	67.944	24.826	1.00	40.04
	1298	CZ	PHE	A	503	20.408	66.829	24.771	1.00	38.82
	1299	N	PHE	A	504	18.967	73.625	24.216	1.00	26.16
	1300	CA	PHE	A	504	18.891	74.988	23.731	1.00	25.00
	1301	C	PHE	A	504	20.182	75.314	23.004	1.00	26.57
	1302	O	PHE	A	504	21.221	74.708	23.267	1.00	26.73
	1303	CB	PHE	A	504	18.640	75.984	24.858	1.00	22.46
	1304	CG	PHE	A	504	19.834	76.270	25.718	1.00	27.70
	1305	CD1	PHE	A	504	20.674	77.340	25.433	1.00	28.94
	1306	CD2	PHE	A	504	20.083	75.514	26.857	1.00	31.34
	1307	CE1	PHE	A	504	21.743	77.662	26.273	1.00	30.08
	1308	CE2	PHE	A	504	21.151	75.828	27.704	1.00	32.65
	1309	CZ	PHE	A	504	21.979	76.909	27.403	1.00	32.80
	1310	N	VAL	A	505	20.091	76.270	22.085	1.00	23.68
	1311	CA	VAL	A	505	21.211	76.705	21.286	1.00	24.67
	1312	C	VAL	A	505	21.041	78.215	21.072	1.00	23.86
	1313	O	VAL	A	505	19.928	78.725	21.049	1.00	21.24
	1314	CB	VAL	A	505	21.208	75.926	19.939	1.00	27.95
	1315	CG1	VAL	A	505	20.134	76.464	19.020	1.00	25.61
	1316	CG2	VAL	A	505	22.558	75.957	19.314	1.00	33.51
	1317	N	PHE	A	506	22.146	78.936	20.959	1.00	26.20
	1318	CA	PHE	A	506	22.086	80.382	20.754	1.00	26.10
	1319	C	PHE	A	506	22.846	80.745	19.479	1.00	24.83
	1320	O	PHE	A	506	23.928	80.231	19.241	1.00	25.52
	1321	CB	PHE	A	506	22.725	81.104	21.939	1.00	28.18
	1322	CG	PHE	A	506	22.758	82.593	21.797	1.00	35.33
	1323	CD1	PHE	A	506	21.620	83.355	22.020	1.00	42.56
	1324	CD2	PHE	A	506	23.937	83.241	21.443	1.00	40.04
	1325	CE1	PHE	A	506	21.660	84.746	21.892	1.00	44.70
	1326	CE2	PHE	A	506	23.987	84.623	21.311	1.00	40.54
	1327	CZ	PHE	A	506	22.851	85.377	21.536	1.00	42.12
	1328	N	SER	A	507	22.290	81.639	18.673	1.00	24.69
	1329	CA	SER	A	507	22.941	82.050	17.426	1.00	24.73
	1330	C	SER	A	507	23.065	83.578	17.355	1.00	26.40
	1331	O	SER	A	507	22.113	84.292	17.609	1.00	25.99
	1332	CB	SER	A	507	22.151	81.521	16.221	1.00	22.19
	1333	OG	SER	A	507	22.740	81.947	15.009	1.00	30.30
	1334	N	ARG	A	508	24.255	84.062	17.009	1.00	26.98
	1335	CA	ARG	A	508	24.545	85.496	16.913	1.00	25.95
	1336	C	ARG	A	508	24.851	85.911	15.463	1.00	24.97
	1337	O	ARG	A	508	25.621	85.250	14.785	1.00	24.35
	1338	CB	ARG	A	508	25.755	85.801	17.790	1.00	21.97
	1339	CG	ARG	A	508	26.249	87.235	17.756	1.00	25.32
	1340	CD	ARG	A	508	27.474	87.372	18.656	1.00	25.67
	1341	NE	ARG	A	508	27.898	88.758	18.788	1.00	36.00
	1342	CZ	ARG	A	508	28.757	89.357	17.972	1.00	36.06
	1343	NH1	ARG	A	508	29.293	88.682	16.963	1.00	34.19

	1344	NH2	ARG	A	508	29.062	90.633	18.157	1.00	34.70
	1345	N	LEU	A	509	24.269	87.017	15.001	1.00	26.44
	1346	CA	LEU	A	509	24.492	87.479	13.621	1.00	28.45
	1347	C	LEU	A	509	24.794	88.973	13.540	1.00	28.87
	1348	O	LEU	A	509	23.893	89.797	13.699	1.00	30.99
	1349	CB	LEU	A	509	23.259	87.177	12.758	1.00	27.28
	1350	CG	LEU	A	509	23.270	87.733	11.321	1.00	31.90
	1351	CD1	LEU	A	509	24.284	86.985	10.453	1.00	29.48
	1352	CD2	LEU	A	509	21.886	87.599	10.732	1.00	28.89
	1353	N	GLU	A	510	26.054	89.323	13.288	1.00	31.92
	1354	CA	GLU	A	510	26.448	90.728	13.189	1.00	34.67
	1355	C	GLU	A	510	26.005	91.290	11.845	1.00	36.35
	1356	O	GLU	A	510	26.199	90.652	10.812	1.00	34.66
	1357	CB	GLU	A	510	27.970	90.875	13.343	1.00	41.07
	1358	CG	GLU	A	510	28.510	90.383	14.696	1.00	54.35
	1359	CD	GLU	A	510	29.997	90.675	14.911	1.00	58.86
	1360	OE1	GLU	A	510	30.811	90.364	14.013	1.00	61.22
	1361	OE2	GLU	A	510	30.349	91.207	15.989	1.00	61.34
	1362	N	VAL	A	511	25.406	92.479	11.852	1.00	36.50
	1363	CA	VAL	A	511	24.935	93.069	10.606	1.00	38.05
	1364	C	VAL	A	511	25.370	94.516	10.408	1.00	42.41
	1365	O	VAL	A	511	25.744	95.205	11.368	1.00	41.92
	1366	CB	VAL	A	511	23.403	93.012	10.508	1.00	31.84
	1367	CG1	VAL	A	511	22.927	91.585	10.669	1.00	32.42
	1368	CG2	VAL	A	511	22.787	93.913	11.553	1.00	26.87
	1369	N	THR	A	512	25.310	94.967	9.154	1.00	43.58
	1370	CA	THR	A	512	25.697	96.331	8.808	1.00	48.37
	1371	C	THR	A	512	24.602	97.306	9.201	1.00	50.53
	1372	O	THR	A	512	23.487	96.894	9.516	1.00	51.77
	1373	CB	THR	A	512	25.956	96.475	7.303	1.00	48.57
	1374	OG1	THR	A	512	24.766	96.140	6.581	1.00	46.96
	1375	CG2	THR	A	512	27.085	95.554	6.866	1.00	45.82
	1376	N	ARG	A	513	24.922	98.598	9.188	1.00	53.29
	1377	CA	ARG	A	513	23.952	99.629	9.544	1.00	55.54
	1378	C	ARG	A	513	22.781	99.557	8.577	1.00	55.38
	1379	O	ARG	A	513	21.623	99.741	8.962	1.00	55.22
	1380	CB	ARG	A	513	24.594	101.018	9.464	1.00	59.23
	1381	CG	ARG	A	513	23.999	102.037	10.428	1.00	65.98
	1382	CD	ARG	A	513	22.519	102.274	10.184	1.00	74.12
	1383	NE	ARG	A	513	21.858	102.827	11.365	1.00	80.97
	1384	CZ	ARG	A	513	20.581	103.197	11.413	1.00	83.64
	1385	NH1	ARG	A	513	19.809	103.084	10.340	1.00	86.02
	1386	NH2	ARG	A	513	20.072	103.673	12.543	1.00	85.44
	1387	N	ALA	A	514	23.099	99.285	7.317	1.00	55.03
	1388	CA	ALA	A	514	22.096	99.186	6.268	1.00	55.46
	1389	C	ALA	A	514	21.061	98.104	6.571	1.00	56.10
	1390	O	ALA	A	514	19.866	98.390	6.674	1.00	56.61
	1391	CB	ALA	A	514	22.775	98.908	4.927	1.00	54.05
	1392	N	GLU	A	515	21.509	96.859	6.712	1.00	55.46
	1393	CA	GLU	A	515	20.575	95.781	6.995	1.00	55.34
	1394	C	GLU	A	515	19.949	95.951	8.371	1.00	54.83
	1395	O	GLU	A	515	18.877	95.410	8.644	1.00	52.33
	1396	CB	GLU	A	515	21.265	94.413	6.868	1.00	57.76
	1397	CG	GLU	A	515	22.716	94.379	7.312	1.00	62.58
	1398	CD	GLU	A	515	23.416	93.082	6.937	1.00	63.27
	1399	OE1	GLU	A	515	23.168	92.565	5.829	1.00	64.89
	1400	OE2	GLU	A	515	24.228	92.586	7.741	1.00	66.59
	1401	N	TRP	A	516	20.608	96.716	9.234	1.00	55.79
	1402	CA	TRP	A	516	20.072	96.956	10.566	1.00	57.81
	1403	C	TRP	A	516	18.818	97.822	10.464	1.00	58.51
	1404	O	TRP	A	516	17.988	97.822	11.374	1.00	57.71
	1405	CB	TRP	A	516	21.101	97.649	11.466	1.00	61.48

	1406	CG	TRP	A	516	20.738	97.544	12.913	1.00	66.54
	1407	CD1	TRP	A	516	20.823	96.428	13.697	1.00	67.26
	1408	CD2	TRP	A	516	20.140	98.561	13.725	1.00	69.56
	1409	NE1	TRP	A	516	20.309	96.685	14.946	1.00	71.76
	1410	CE2	TRP	A	516	19.882	97.987	14.990	1.00	70.88
	1411	CE3	TRP	A	516	19.793	99.900	13.507	1.00	70.94
	1412	CZ2	TRP	A	516	19.292	98.706	16.034	1.00	73.50
	1413	CZ3	TRP	A	516	19.204	100.618	14.548	1.00	74.37
	1414	CH2	TRP	A	516	18.961	100.016	15.796	1.00	74.71
	1415	N	GLU	A	517	18.682	98.553	9.356	1.00	59.66
	1416	CA	GLU	A	517	17.515	99.409	9.128	1.00	61.72
	1417	C	GLU	A	517	16.301	98.565	8.746	1.00	59.87
	1418	O	GLU	A	517	15.159	98.994	8.904	1.00	58.60
	1419	CB	GLU	A	517	17.782	100.418	8.003	1.00	68.82
	1420	CG	GLU	A	517	18.988	101.316	8.221	1.00	80.60
	1421	CD	GLU	A	517	19.148	102.358	7.124	1.00	87.42
	1422	OE1	GLU	A	517	18.472	102.231	6.079	1.00	94.80
	1423	OE2	GLU	A	517	19.955	103.299	7.300	1.00	95.35
	1424	N	GLN	A	518	16.555	97.366	8.233	1.00	57.92
	1425	CA	GLN	A	518	15.480	96.468	7.836	1.00	55.74
	1426	C	GLN	A	518	15.543	95.184	8.664	1.00	54.32
	1427	O	GLN	A	518	15.207	94.102	8.176	1.00	52.85
	1428	CB	GLN	A	518	15.600	96.146	6.355	1.00	54.10
	1429	N	LYS	A	519	15.954	95.313	9.924	1.00	52.69
	1430	CA	LYS	A	519	16.082	94.152	10.791	1.00	52.35
	1431	C	LYS	A	519	14.781	93.394	10.941	1.00	51.69
	1432	O	LYS	A	519	14.778	92.203	11.246	1.00	49.61
	1433	CB	LYS	A	519	16.617	94.561	12.163	1.00	54.31
	1434	CG	LYS	A	519	15.688	95.395	13.012	1.00	55.80
	1435	CD	LYS	A	519	16.438	95.877	14.241	1.00	60.32
	1436	CE	LYS	A	519	15.598	96.806	15.089	1.00	64.05
	1437	NZ	LYS	A	519	16.409	97.377	16.202	1.00	70.92
	1438	N	ASP	A	520	13.676	94.089	10.712	1.00	52.66
	1439	CA	ASP	A	520	12.349	93.495	10.812	1.00	54.22
	1440	C	ASP	A	520	12.204	92.391	9.764	1.00	53.07
	1441	O	ASP	A	520	11.336	91.525	9.871	1.00	52.75
	1442	CB	ASP	A	520	11.289	94.568	10.563	1.00	61.14
	1443	CG	ASP	A	520	11.821	95.980	10.792	1.00	71.19
	1444	OD1	ASP	A	520	12.193	96.300	11.945	1.00	76.53
	1445	OD2	ASP	A	520	11.871	96.766	9.817	1.00	72.86
	1446	N	GLU	A	521	13.067	92.423	8.757	1.00	51.01
	1447	CA	GLU	A	521	13.018	91.443	7.684	1.00	50.49
	1448	C	GLU	A	521	13.886	90.206	7.899	1.00	47.73
	1449	O	GLU	A	521	13.762	89.228	7.165	1.00	48.58
	1450	CB	GLU	A	521	13.400	92.107	6.362	1.00	53.54
	1451	CG	GLU	A	521	12.423	93.173	5.901	1.00	60.11
	1452	CD	GLU	A	521	12.901	93.895	4.658	1.00	65.41
	1453	OE1	GLU	A	521	13.103	93.239	3.614	1.00	67.98
	1454	OE2	GLU	A	521	13.079	95.129	4.726	1.00	73.58
	1455	N	PHE	A	522	14.772	90.241	8.887	1.00	42.66
	1456	CA	PHE	A	522	15.615	89.081	9.137	1.00	38.90
	1457	C	PHE	A	522	14.847	88.017	9.892	1.00	35.93
	1458	O	PHE	A	522	14.021	88.324	10.755	1.00	38.85
	1459	CB	PHE	A	522	16.884	89.478	9.886	1.00	36.56
	1460	CG	PHE	A	522	17.890	90.181	9.019	1.00	39.04
	1461	CD1	PHE	A	522	17.673	91.494	8.605	1.00	42.28
	1462	CD2	PHE	A	522	19.026	89.513	8.561	1.00	36.78
	1463	CE1	PHE	A	522	18.571	92.132	7.738	1.00	44.30
	1464	CE2	PHE	A	522	19.927	90.139	7.695	1.00	40.92
	1465	CZ	PHE	A	522	19.699	91.454	7.283	1.00	39.51
	1466	N	ILE	A	523	15.108	86.763	9.545	1.00	31.27
	1467	CA	ILE	A	523	14.427	85.641	10.156	1.00	29.65

	1468	C	ILE	A	523	15.389	84.551	10.617	1.00	29.13
	1469	O	ILE	A	523	16.364	84.240	9.936	1.00	27.36
	1470	CB	ILE	A	523	13.420	85.033	9.163	1.00	34.21
	1471	CG1	ILE	A	523	12.349	86.072	8.818	1.00	37.38
	1472	CG2	ILE	A	523	12.804	83.773	9.736	1.00	34.94
	1473	CD1	ILE	A	523	11.373	85.619	7.746	1.00	38.56
	1474	N	CYS	A	524	15.102	83.990	11.789	1.00	26.34
	1475	CA	CYS	A	524	15.901	82.914	12.361	1.00	27.10
	1476	C	CYS	A	524	15.100	81.654	12.138	1.00	26.67
	1477	O	CYS	A	524	13.945	81.590	12.531	1.00	27.58
	1478	CB	CYS	A	524	16.103	83.127	13.874	1.00	24.27
	1479	SG	CYS	A	524	16.974	81.777	14.737	1.00	37.60
	1480	N	ARG	A	525	15.714	80.649	11.528	1.00	26.37
	1481	CA	ARG	A	525	15.024	79.406	11.244	1.00	26.35
	1482	C	ARG	A	525	15.713	78.181	11.796	1.00	26.72
	1483	O	ARG	A	525	16.929	78.039	11.700	1.00	29.04
	1484	CB	ARG	A	525	14.852	79.224	9.739	1.00	29.81
	1485	CG	ARG	A	525	14.207	77.887	9.372	1.00	35.40
	1486	CD	ARG	A	525	13.542	77.948	8.001	1.00	46.51
	1487	NE	ARG	A	525	14.487	77.804	6.907	1.00	50.77
	1488	CZ	ARG	A	525	14.221	78.139	5.649	1.00	55.09
	1489	NH1	ARG	A	525	13.035	78.649	5.337	1.00	54.58
	1490	NH2	ARG	A	525	15.136	77.950	4.703	1.00	56.77
	1491	N	ALA	A	526	14.920	77.289	12.369	1.00	25.38
	1492	CA	ALA	A	526	15.458	76.072	12.920	1.00	25.38
	1493	C	ALA	A	526	14.872	74.879	12.175	1.00	25.99
	1494	O	ALA	A	526	13.667	74.849	11.890	1.00	25.50
	1495	CB	ALA	A	526	15.116	75.971	14.404	1.00	25.98
	1496	N	VAL	A	527	15.728	73.916	11.841	1.00	23.84
	1497	CA	VAL	A	527	15.267	72.705	11.198	1.00	25.15
	1498	C	VAL	A	527	15.522	71.628	12.220	1.00	26.30
	1499	O	VAL	A	527	16.642	71.481	12.706	1.00	26.20
	1500	CB	VAL	A	527	16.043	72.365	9.923	1.00	24.43
	1501	CG1	VAL	A	527	15.610	71.012	9.439	1.00	26.95
	1502	CG2	VAL	A	527	15.781	73.409	8.849	1.00	28.13
	1503	N	HIS	A	528	14.485	70.862	12.531	1.00	26.24
	1504	CA	HIS	A	528	14.582	69.828	13.536	1.00	29.14
	1505	C	HIS	A	528	13.498	68.778	13.295	1.00	31.86
	1506	O	HIS	A	528	12.384	69.091	12.861	1.00	31.05
	1507	CB	HIS	A	528	14.428	70.479	14.921	1.00	29.03
	1508	CG	HIS	A	528	14.518	69.523	16.065	1.00	29.34
	1509	ND1	HIS	A	528	13.491	68.666	16.404	1.00	33.33
	1510	CD2	HIS	A	528	15.510	69.283	16.956	1.00	28.93
	1511	CE1	HIS	A	528	13.845	67.945	17.449	1.00	26.07
	1512	NE2	HIS	A	528	15.070	68.298	17.805	1.00	32.19
	1513	N	GLU	A	529	13.843	67.536	13.599	1.00	34.08
	1514	CA	GLU	A	529	12.964	66.393	13.424	1.00	39.76
	1515	C	GLU	A	529	11.563	66.490	14.034	1.00	41.50
	1516	O	GLU	A	529	10.580	66.190	13.360	1.00	41.48
	1517	CB	GLU	A	529	13.641	65.138	13.978	1.00	43.03
	1518	CG	GLU	A	529	12.702	63.935	14.014	1.00	56.19
	1519	CD	GLU	A	529	13.239	62.773	14.826	1.00	62.66
	1520	OE1	GLU	A	529	12.489	61.788	15.007	1.00	63.52
	1521	OE2	GLU	A	529	14.402	62.842	15.281	1.00	65.43
	1522	N	ALA	A	530	11.479	66.897	15.300	1.00	42.51
	1523	CA	ALA	A	530	10.201	66.978	16.006	1.00	46.03
	1524	C	ALA	A	530	9.269	68.105	15.596	1.00	49.29
	1525	O	ALA	A	530	8.124	68.153	16.044	1.00	50.87
	1526	CB	ALA	A	530	10.443	67.043	17.513	1.00	39.71
	1527	N	ALA	A	531	9.751	69.005	14.748	1.00	52.89
	1528	CA	ALA	A	531	8.949	70.133	14.302	1.00	56.14
	1529	C	ALA	A	531	8.030	69.799	13.124	1.00	59.66

1530	O	ALA	A	531	8.258	70.243	12.004	1.00	61.00
1531	CB	ALA	A	531	9.864	71.295	13.938	1.00	52.83
1532	N	SER	A	532	6.992	69.012	13.370	1.00	63.07
1533	CA	SER	A	532	6.056	68.673	12.305	1.00	66.03
1534	C	SER	A	532	5.006	69.778	12.250	1.00	66.08
1535	O	SER	A	532	4.569	70.283	13.286	1.00	65.35
1536	CB	SER	A	532	5.384	67.330	12.593	1.00	68.98
1537	OG	SER	A	532	4.526	67.416	13.716	1.00	74.64
1538	N	PRO	A	533	4.581	70.173	11.043	1.00	66.51
1539	CA	PRO	A	533	4.931	69.713	9.696	1.00	65.99
1540	C	PRO	A	533	6.251	70.226	9.117	1.00	63.48
1541	O	PRO	A	533	6.760	71.273	9.518	1.00	64.33
1542	CB	PRO	A	533	3.757	70.203	8.873	1.00	69.06
1543	CG	PRO	A	533	3.539	71.556	9.471	1.00	71.08
1544	CD	PRO	A	533	3.570	71.242	10.963	1.00	70.23
1545	N	SER	A	534	6.783	69.466	8.165	1.00	59.21
1546	CA	SER	A	534	8.009	69.804	7.452	1.00	55.01
1547	C	SER	A	534	9.274	70.148	8.248	1.00	50.27
1548	O	SER	A	534	10.130	70.875	7.753	1.00	48.58
1549	CB	SER	A	534	7.706	70.934	6.475	1.00	58.20
1550	OG	SER	A	534	7.074	72.013	7.138	1.00	63.36
1551	N	GLN	A	535	9.387	69.616	9.461	1.00	44.89
1552	CA	GLN	A	535	10.543	69.829	10.330	1.00	42.88
1553	C	GLN	A	535	11.194	71.205	10.277	1.00	41.55
1554	O	GLN	A	535	12.419	71.321	10.294	1.00	40.80
1555	CB	GLN	A	535	11.633	68.769	10.080	1.00	37.08
1556	CG	GLN	A	535	11.302	67.731	9.056	1.00	47.40
1557	CD	GLN	A	535	10.101	66.916	9.431	1.00	44.36
1558	OE1	GLN	A	535	9.193	66.738	8.625	1.00	47.59
1559	NE2	GLN	A	535	10.079	66.415	10.664	1.00	54.70
1560	N	THR	A	536	10.387	72.252	10.226	1.00	39.97
1561	CA	THR	A	536	10.950	73.588	10.207	1.00	40.62
1562	C	THR	A	536	10.113	74.575	11.023	1.00	37.57
1563	O	THR	A	536	8.893	74.558	10.975	1.00	40.85
1564	CB	THR	A	536	11.137	74.092	8.747	1.00	42.38
1565	OG1	THR	A	536	11.458	75.488	8.763	1.00	44.59
1566	CG2	THR	A	536	9.881	73.870	7.932	1.00	49.65
1567	N	VAL	A	537	10.788	75.410	11.801	1.00	35.29
1568	CA	VAL	A	537	10.147	76.418	12.632	1.00	31.25
1569	C	VAL	A	537	10.996	77.678	12.537	1.00	29.01
1570	O	VAL	A	537	12.218	77.615	12.699	1.00	30.11
1571	CB	VAL	A	537	10.106	75.996	14.117	1.00	34.80
1572	CG1	VAL	A	537	9.452	77.084	14.939	1.00	35.52
1573	CG2	VAL	A	537	9.341	74.712	14.278	1.00	37.19
1574	N	GLN	A	538	10.365	78.820	12.292	1.00	26.73
1575	CA	GLN	A	538	11.107	80.067	12.167	1.00	26.74
1576	C	GLN	A	538	10.376	81.271	12.732	1.00	27.53
1577	O	GLN	A	538	9.169	81.249	12.902	1.00	29.89
1578	CB	GLN	A	538	11.424	80.335	10.700	1.00	28.48
1579	CG	GLN	A	538	10.208	80.624	9.834	1.00	25.88
1580	CD	GLN	A	538	10.595	80.853	8.378	1.00	28.51
1581	OE1	GLN	A	538	11.390	80.102	7.810	1.00	31.66
1582	NE2	GLN	A	538	10.035	81.885	7.772	1.00	27.39
1583	N	ARG	A	539	11.113	82.334	13.013	1.00	28.05
1584	CA	ARG	A	539	10.493	83.530	13.535	1.00	30.72
1585	C	ARG	A	539	11.288	84.742	13.114	1.00	31.33
1586	O	ARG	A	539	12.517	84.703	13.077	1.00	32.42
1587	CB	ARG	A	539	10.420	83.463	15.061	1.00	36.30
1588	CG	ARG	A	539	9.488	84.476	15.686	1.00	45.60
1589	CD	ARG	A	539	8.741	83.829	16.830	1.00	57.97
1590	NE	ARG	A	539	8.118	82.591	16.371	1.00	69.46
1591	CZ	ARG	A	539	7.453	81.745	17.150	1.00	78.18

	1592	NH1	ARG	A	539	7.316	81.996	18.447	1.00	83.01
	1593	NH2	ARG	A	539	6.927	80.641	16.630	1.00	81.89
	1594	N	ALA	A	540	10.578	85.818	12.799	1.00	31.92
	1595	CA	ALA	A	540	11.207	87.054	12.383	1.00	34.50
	1596	C	ALA	A	540	11.691	87.774	13.634	1.00	36.68
	1597	O	ALA	A	540	11.190	87.532	14.739	1.00	34.62
	1598	CB	ALA	A	540	10.209	87.907	11.621	1.00	33.91
	1599	N	VAL	A	541	12.694	88.626	13.460	1.00	39.73
	1600	CA	VAL	A	541	13.254	89.386	14.572	1.00	44.47
	1601	C	VAL	A	541	12.164	90.249	15.218	1.00	46.91
	1602	O	VAL	A	541	11.595	91.124	14.573	1.00	44.53
	1603	CB	VAL	A	541	14.415	90.295	14.090	1.00	42.49
	1604	CG1	VAL	A	541	14.715	91.358	15.130	1.00	47.96
	1605	CG2	VAL	A	541	15.655	89.460	13.831	1.00	42.43
	1606	N	SER	A	542	11.869	89.997	16.489	1.00	52.25
	1607	CA	SER	A	542	10.840	90.771	17.174	1.00	60.05
	1608	C	SER	A	542	11.374	92.174	17.421	1.00	64.25
	1609	O	SER	A	542	12.550	92.353	17.743	1.00	65.22
	1610	CB	SER	A	542	10.443	90.110	18.500	1.00	60.43
	1611	OG	SER	A	542	11.530	90.076	19.404	1.00	65.30
	1612	N	VAL	A	543	10.510	93.168	17.256	1.00	68.19
	1613	CA	VAL	A	543	10.906	94.557	17.444	1.00	72.45
	1614	C	VAL	A	543	9.828	95.323	18.202	1.00	74.32
	1615	O	VAL	A	543	8.970	95.979	17.603	1.00	75.99
	1616	CB	VAL	A	543	11.148	95.247	16.084	1.00	74.41
	1617	CG1	VAL	A	543	11.530	96.705	16.299	1.00	76.37
	1618	CG2	VAL	A	543	12.233	94.514	15.318	1.00	75.78
	1619	N	VAL	B	336	42.982	59.443	29.109	1.00	58.93
	1620	CA	VAL	B	336	43.788	60.200	30.107	1.00	60.44
	1621	C	VAL	B	336	44.173	61.587	29.599	1.00	60.07
	1622	O	VAL	B	336	45.211	61.753	28.958	1.00	61.48
	1623	CB	VAL	B	336	45.079	59.445	30.453	1.00	60.81
	1624	CG1	VAL	B	336	45.794	60.136	31.600	1.00	61.71
	1625	CG2	VAL	B	336	44.755	58.010	30.798	1.00	64.73
	1626	N	SER	B	337	43.343	62.583	29.891	1.00	57.95
	1627	CA	SER	B	337	43.617	63.945	29.452	1.00	56.60
	1628	C	SER	B	337	43.758	64.917	30.624	1.00	55.17
	1629	O	SER	B	337	43.338	64.619	31.748	1.00	54.55
	1630	CB	SER	B	337	42.522	64.415	28.497	1.00	57.92
	1631	OG	SER	B	337	41.244	64.111	29.013	1.00	64.70
	1632	N	ALA	B	338	44.362	66.073	30.357	1.00	52.40
	1633	CA	ALA	B	338	44.590	67.078	31.389	1.00	50.69
	1634	C	ALA	B	338	44.300	68.491	30.908	1.00	50.25
	1635	O	ALA	B	338	44.538	68.828	29.746	1.00	51.17
	1636	CB	ALA	B	338	46.027	66.989	31.889	1.00	50.21
	1637	N	TYR	B	339	43.792	69.319	31.816	1.00	48.22
	1638	CA	TYR	B	339	43.461	70.701	31.495	1.00	46.82
	1639	C	TYR	B	339	43.834	71.610	32.669	1.00	44.51
	1640	O	TYR	B	339	43.711	71.228	33.832	1.00	42.27
	1641	CB	TYR	B	339	41.962	70.835	31.185	1.00	50.52
	1642	CG	TYR	B	339	41.402	69.731	30.307	1.00	58.40
	1643	CD1	TYR	B	339	41.155	68.456	30.826	1.00	61.23
	1644	CD2	TYR	B	339	41.144	69.952	28.949	1.00	60.99
	1645	CE1	TYR	B	339	40.671	67.426	30.019	1.00	62.71
	1646	CE2	TYR	B	339	40.657	68.926	28.131	1.00	63.53
	1647	CZ	TYR	B	339	40.424	67.667	28.673	1.00	64.33
	1648	OH	TYR	B	339	39.956	66.647	27.870	1.00	65.07
	1649	N	LEU	B	340	44.309	72.807	32.354	1.00	41.90

	1650	CA	LEU	B	340	44.695	73.769	33.372	1.00	41.06
	1651	C	LEU	B	340	43.929	75.029	33.022	1.00	41.10
5	1652	O	LEU	B	340	43.953	75.464	31.876	1.00	43.45
	1653	CB	LEU	B	340	46.208	74.017	33.321	1.00	36.93
	1654	CG	LEU	B	340	46.830	74.911	34.399	1.00	35.91
	1655	CD1	LEU	B	340	46.500	74.371	35.786	1.00	34.60
	1656	CD2	LEU	B	340	48.336	74.979	34.194	1.00	35.51
10	1657	N	SER	B	341	43.232	75.610	33.992	1.00	39.82
	1658	CA	SER	B	341	42.448	76.810	33.715	1.00	39.85
	1659	C	SER	B	341	42.955	78.002	34.486	1.00	37.88
	1660	O	SER	B	341	43.524	77.863	35.556	1.00	42.10
	1661	CB	SER	B	341	40.973	76.575	34.058	1.00	39.34
15	1662	OG	SER	B	341	40.808	76.253	35.428	1.00	44.58
	1663	N	ARG	B	342	42.732	79.185	33.942	1.00	36.98
	1664	CA	ARG	B	342	43.163	80.413	34.583	1.00	35.20
	1665	C	ARG	B	342	42.183	80.747	35.707	1.00	33.18
	1666	O	ARG	B	342	41.157	80.092	35.848	1.00	33.16
20	1667	CB	ARG	B	342	43.206	81.530	33.534	1.00	38.57
	1668	CG	ARG	B	342	44.219	81.279	32.411	1.00	39.10
	1669	CD	ARG	B	342	44.236	82.409	31.388	1.00	43.21
	1670	NE	ARG	B	342	43.056	82.369	30.530	1.00	45.40
	1671	CZ	ARG	B	342	42.886	81.514	29.527	1.00	48.22
25	1672	NH1	ARG	B	342	43.823	80.623	29.240	1.00	52.78
	1673	NH2	ARG	B	342	41.769	81.541	28.814	1.00	54.34
	1674	N	PRO	B	343	42.488	81.757	36.530	1.00	33.03
	1675	CA	PRO	B	343	41.560	82.103	37.619	1.00	34.14
	1676	C	PRO	B	343	40.261	82.693	37.065	1.00	34.06
30	1677	O	PRO	B	343	40.259	83.298	35.994	1.00	35.44
	1678	CB	PRO	B	343	42.334	83.152	38.433	1.00	32.07
	1679	CG	PRO	B	343	43.789	82.900	38.075	1.00	35.06
	1680	CD	PRO	B	343	43.715	82.571	36.601	1.00	33.27
	1681	N	SER	B	344	39.155	82.520	37.775	1.00	32.17
35	1682	CA	SER	B	344	37.909	83.110	37.308	1.00	31.75
	1683	C	SER	B	344	37.983	84.586	37.686	1.00	32.07
	1684	O	SER	B	344	38.485	84.940	38.756	1.00	30.21
	1685	CB	SER	B	344	36.693	82.456	37.982	1.00	32.20
	1686	OG	SER	B	344	36.487	82.935	39.301	1.00	32.50
40	1687	N	PRO	B	345	37.512	85.473	36.800	1.00	32.31
	1688	CA	PRO	B	345	37.561	86.899	37.125	1.00	30.84
	1689	C	PRO	B	345	36.890	87.219	38.471	1.00	29.64
	1690	O	PRO	B	345	37.344	88.094	39.209	1.00	30.14
	1691	CB	PRO	B	345	36.859	87.545	35.926	1.00	30.96
45	1692	CG	PRO	B	345	37.299	86.659	34.793	1.00	33.18
	1693	CD	PRO	B	345	37.143	85.261	35.387	1.00	33.65
	1694	N	PHE	B	346	35.831	86.497	38.808	1.00	28.34
	1695	CA	PHE	B	346	35.153	86.756	40.066	1.00	31.46
	1696	C	PHE	B	346	36.078	86.515	41.269	1.00	32.46
50	1697	O	PHE	B	346	36.135	87.331	42.193	1.00	32.59
	1698	CB	PHE	B	346	33.894	85.889	40.184	1.00	32.72
	1699	CG	PHE	B	346	33.218	85.987	41.521	1.00	36.34
	1700	CD1	PHE	B	346	32.619	87.170	41.928	1.00	40.58
	1701	CD2	PHE	B	346	33.189	84.898	42.378	1.00	36.76
55	1702	CE1	PHE	B	346	31.991	87.267	43.167	1.00	38.98
	1703	CE2	PHE	B	346	32.563	84.985	43.618	1.00	40.15
	1704	CZ	PHE	B	346	31.963	86.175	44.014	1.00	38.60
	1705	N	ASP	B	347	36.803	85.397	41.250	1.00	32.92
	1706	CA	ASP	B	347	37.723	85.066	42.336	1.00	33.58
5	1707	C	ASP	B	347	38.896	86.045	42.367	1.00	34.26
	1708	O	ASP	B	347	39.388	86.408	43.434	1.00	32.29
	1709	CB	ASP	B	347	38.251	83.633	42.179	1.00	28.72
	1710	CG	ASP	B	347	37.236	82.592	42.579	1.00	39.62
	1711	OD1	ASP	B	347	37.515	81.375	42.429	1.00	42.08

	1712	OD2	ASP	B	347	36.151	82.991	43.054	1.00	46.23
	1713	N	LEU	B	348	39.324	86.480	41.189	1.00	34.31
	1714	CA	LEU	B	348	40.441	87.403	41.064	1.00	37.70
	1715	C	LEU	B	348	40.159	88.858	41.471	1.00	38.98
	1716	O	LEU	B	348	40.949	89.463	42.198	1.00	38.11
	1717	CB	LEU	B	348	40.959	87.380	39.618	1.00	40.66
	1718	CG	LEU	B	348	42.159	88.267	39.260	1.00	41.99
	1719	CD1	LEU	B	348	43.388	87.862	40.095	1.00	42.77
	1720	CD2	LEU	B	348	42.469	88.124	37.759	1.00	41.00
	1721	N	PHE	B	349	39.040	89.417	41.017	1.00	39.68
	1722	CA	PHE	B	349	38.725	90.819	41.306	1.00	42.09
	1723	C	PHE	B	349	37.717	91.134	42.405	1.00	45.09
	1724	O	PHE	B	349	37.821	92.169	43.062	1.00	48.27
	1725	CB	PHE	B	349	38.272	91.526	40.029	1.00	37.36
	1726	CG	PHE	B	349	39.244	91.411	38.900	1.00	36.93
	1727	CD1	PHE	B	349	38.976	90.579	37.818	1.00	38.16
	1728	CD2	PHE	B	349	40.444	92.113	38.926	1.00	38.04
	1729	CE1	PHE	B	349	39.885	90.445	36.781	1.00	38.11
	1730	CE2	PHE	B	349	41.369	91.986	37.887	1.00	37.58
	1731	CZ	PHE	B	349	41.089	91.151	36.817	1.00	40.39
	1732	N	ILE	B	350	36.726	90.277	42.600	1.00	46.66
	1733	CA	ILE	B	350	35.746	90.548	43.639	1.00	48.94
	1734	C	ILE	B	350	36.200	89.905	44.950	1.00	51.15
	1735	O	ILE	B	350	36.505	90.593	45.921	1.00	50.51
	1736	CB	ILE	B	350	34.359	90.008	43.240	1.00	48.52
	1737	CG1	ILE	B	350	34.038	90.428	41.801	1.00	49.25
	1738	CG2	ILE	B	350	33.300	90.548	44.177	1.00	49.68
	1739	CD1	ILE	B	350	34.242	91.911	41.533	1.00	46.80
	1740	N	ARG	B	351	36.265	88.579	44.945	1.00	52.64
	1741	CA	ARG	B	351	36.669	87.793	46.100	1.00	53.76
	1742	C	ARG	B	351	38.114	88.090	46.519	1.00	53.61
	1743	O	ARG	B	351	38.436	88.094	47.703	1.00	53.55
	1744	CB	ARG	B	351	36.505	86.313	45.759	1.00	56.64
	1745	CG	ARG	B	351	36.016	85.434	46.894	1.00	62.18
	1746	CD	ARG	B	351	35.073	84.375	46.348	1.00	66.96
	1747	NE	ARG	B	351	34.958	83.211	47.219	1.00	71.13
	1748	CZ	ARG	B	351	35.957	82.371	47.470	1.00	76.72
	1749	NH1	ARG	B	351	37.145	82.573	46.916	1.00	78.73
	1750	NH2	ARG	B	351	35.771	81.325	48.268	1.00	77.63
	1751	N	LYS	B	352	38.974	88.347	45.540	1.00	53.86
	1752	CA	LYS	B	352	40.385	88.646	45.788	1.00	54.12
	1753	C	LYS	B	352	41.172	87.449	46.328	1.00	52.02
	1754	O	LYS	B	352	42.078	87.604	47.146	1.00	51.77
	1755	CB	LYS	B	352	40.525	89.825	46.753	1.00	57.77
	1756	CG	LYS	B	352	39.911	91.124	46.254	1.00	62.15
	1757	CD	LYS	B	352	40.161	92.252	47.254	1.00	71.06
	1758	CE	LYS	B	352	39.351	93.502	46.929	1.00	74.25
	1759	NZ	LYS	B	352	37.893	93.307	47.185	1.00	78.35
	1760	N	SER	B	353	40.811	86.258	45.867	1.00	48.01
	1761	CA	SER	B	353	41.488	85.032	46.268	1.00	45.29
	1762	C	SER	B	353	41.446	84.056	45.084	1.00	40.67
	1763	O	SER	B	353	40.725	83.054	45.106	1.00	40.76
	1764	CB	SER	B	353	40.809	84.423	47.498	1.00	47.97
	1765	OG	SER	B	353	39.445	84.152	47.247	1.00	56.20
	1766	N	PRO	B	354	42.225	84.356	44.030	1.00	36.53
	1767	CA	PRO	B	354	42.361	83.596	42.781	1.00	32.68
	1768	C	PRO	B	354	42.940	82.201	42.961	1.00	31.88
	1769	O	PRO	B	354	43.813	81.985	43.798	1.00	29.76
	1770	CB	PRO	B	354	43.306	84.453	41.940	1.00	30.29
	1771	CG	PRO	B	354	43.260	85.801	42.587	1.00	41.68
	1772	CD	PRO	B	354	43.155	85.494	44.035	1.00	33.29
	1773	N	THR	B	355	42.446	81.258	42.168	1.00	30.03

	1774	CA	THR	B	355	42.956	79.896	42.198	1.00	29.70
	1775	C	THR	B	355	43.022	79.364	40.774	1.00	30.82
	1776	O	THR	B	355	42.302	79.827	39.887	1.00	30.67
	1777	CB	THR	B	355	42.042	78.931	42.964	1.00	32.14
	1778	OG1	THR	B	355	40.815	78.794	42.240	1.00	29.97
	1779	CG2	THR	B	355	41.763	79.425	44.393	1.00	31.76
	1780	N	ILE	B	356	43.907	78.405	40.542	1.00	30.53
	1781	CA	ILE	B	356	43.969	77.784	39.232	1.00	31.56
	1782	C	ILE	B	356	43.740	76.321	39.525	1.00	31.79
	1783	O	ILE	B	356	44.039	75.848	40.625	1.00	30.35
	1784	CB	ILE	B	356	45.315	78.016	38.517	1.00	30.05
	1785	CG1	ILE	B	356	46.467	77.499	39.371	1.00	31.32
	1786	CG2	ILE	B	356	45.469	79.508	38.210	1.00	31.27
	1787	CD1	ILE	B	356	47.828	77.757	38.763	1.00	36.89
	1788	N	THR	B	357	43.198	75.605	38.550	1.00	33.31
	1789	CA	THR	B	357	42.881	74.205	38.751	1.00	33.68
	1790	C	THR	B	357	43.403	73.318	37.644	1.00	35.47
	1791	O	THR	B	357	43.228	73.607	36.459	1.00	36.65
	1792	CB	THR	B	357	41.335	74.011	38.855	1.00	33.81
	1793	OG1	THR	B	357	40.844	74.683	40.023	1.00	33.71
	1794	CG2	THR	B	357	40.968	72.535	38.921	1.00	29.63
	1795	N	CYS	B	358	44.034	72.228	38.048	1.00	35.41
	1796	CA	CYS	B	358	44.561	71.254	37.110	1.00	38.12
	1797	C	CYS	B	358	43.570	70.093	37.165	1.00	37.77
	1798	O	CYS	B	358	43.395	69.473	38.210	1.00	36.67
	1799	CB	CYS	B	358	45.945	70.789	37.568	1.00	40.37
	1800	SG	CYS	B	358	46.871	69.769	36.374	1.00	49.83
	1801	N	LEU	B	359	42.909	69.822	36.046	1.00	39.77
	1802	CA	LEU	B	359	41.932	68.747	35.973	1.00	42.86
	1803	C	LEU	B	359	42.432	67.593	35.123	1.00	46.01
	1804	O	LEU	B	359	42.748	67.769	33.948	1.00	47.43
	1805	CB	LEU	B	359	40.612	69.265	35.389	1.00	42.74
	1806	CG	LEU	B	359	39.604	68.208	34.904	1.00	45.03
	1807	CD1	LEU	B	359	39.252	67.338	36.057	1.00	47.59
	1808	CD2	LEU	B	359	38.403	68.889	34.262	1.00	47.51
	1809	N	VAL	B	360	42.493	66.411	35.721	1.00	48.26
	1810	CA	VAL	B	360	42.931	65.220	35.010	1.00	52.34
	1811	C	VAL	B	360	41.765	64.243	34.883	1.00	55.48
	1812	O	VAL	B	360	41.092	63.928	35.866	1.00	55.57
	1813	CB	VAL	B	360	44.100	64.527	35.747	1.00	53.36
	1814	CG1	VAL	B	360	44.482	63.240	35.029	1.00	51.62
	1815	CG2	VAL	B	360	45.299	65.467	35.816	1.00	51.77
	1816	N	VAL	B	361	41.520	63.773	33.665	1.00	58.92
	1817	CA	VAL	B	361	40.433	62.834	33.416	1.00	63.13
	1818	C	VAL	B	361	40.993	61.506	32.926	1.00	67.77
	1819	O	VAL	B	361	41.738	61.466	31.946	1.00	68.38
	1820	CB	VAL	B	361	39.442	63.377	32.353	1.00	60.50
	1821	CG1	VAL	B	361	38.358	62.355	32.086	1.00	56.92
	1822	CG2	VAL	B	361	38.814	64.671	32.830	1.00	56.10
	1823	N	ASP	B	362	40.635	60.426	33.615	1.00	72.90
	1824	CA	ASP	B	362	41.098	59.085	33.259	1.00	78.30
	1825	C	ASP	B	362	39.904	58.244	32.816	1.00	81.68
	1826	O	ASP	B	362	39.168	57.709	33.648	1.00	81.72
	1827	CB	ASP	B	362	41.771	58.415	34.462	1.00	80.22
	1828	CG	ASP	B	362	42.530	57.156	34.080	1.00	84.67
	1829	OD1	ASP	B	362	42.113	56.478	33.117	1.00	87.54
	1830	OD2	ASP	B	362	43.537	56.837	34.749	1.00	87.19
	1831	N	LEU	B	363	39.723	58.126	31.503	1.00	85.84
	1832	CA	LEU	B	363	38.614	57.366	30.935	1.00	89.95
	1833	C	LEU	B	363	38.562	55.923	31.428	1.00	92.20
	1834	O	LEU	B	363	37.483	55.386	31.668	1.00	92.55
	1835	CB	LEU	B	363	38.694	57.390	29.409	1.00	91.66

	1836	CG	LEU	B	363	38.719	58.777	28.758	1.00	92.93
	1837	CD1	LEU	B	363	38.813	58.624	27.246	1.00	95.41
	1838	CD2	LEU	B	363	37.471	59.551	29.137	1.00	92.73
	1839	N	ALA	B	364	39.726	55.296	31.573	1.00	94.76
	1840	CA	ALA	B	364	39.801	53.916	32.051	1.00	97.66
	1841	C	ALA	B	364	40.794	53.831	33.210	1.00	99.72
	1842	O	ALA	B	364	41.998	53.996	33.021	1.00	100.44
	1843	CB	ALA	B	364	40.235	52.996	30.921	1.00	97.99
	1844	N	PRO	B	365	40.297	53.577	34.429	1.00	101.15
	1845	CA	PRO	B	365	41.173	53.484	35.602	1.00	102.25
	1846	C	PRO	B	365	41.895	52.163	35.855	1.00	103.43
	1847	O	PRO	B	365	41.274	51.103	35.934	1.00	104.19
	1848	CB	PRO	B	365	40.237	53.829	36.761	1.00	101.91
	1849	CG	PRO	B	365	39.121	54.617	36.098	1.00	102.27
	1850	CD	PRO	B	365	38.910	53.833	34.846	1.00	101.40
	1851	N	SER	B	366	43.215	52.256	35.979	1.00	104.18
	1852	CA	SER	B	366	44.088	51.132	36.299	1.00	104.43
	1853	C	SER	B	366	44.573	51.676	37.637	1.00	104.05
	1854	O	SER	B	366	44.888	52.864	37.727	1.00	104.36
	1855	CB	SER	B	366	45.249	51.055	35.312	1.00	105.50
	1856	OG	SER	B	366	46.040	52.223	35.413	1.00	106.70
	1857	N	LYS	B	367	44.645	50.861	38.682	1.00	103.19
	1858	CA	LYS	B	367	45.041	51.462	39.944	1.00	102.08
	1859	C	LYS	B	367	46.491	51.630	40.367	1.00	100.74
	1860	O	LYS	B	367	47.234	50.683	40.640	1.00	101.05
	1861	CB	LYS	B	367	44.236	50.868	41.102	1.00	103.30
	1862	CG	LYS	B	367	44.343	49.384	41.345	1.00	105.00
	1863	CD	LYS	B	367	43.374	49.046	42.467	1.00	104.80
	1864	CE	LYS	B	367	43.467	47.610	42.930	1.00	104.70
	1865	NZ	LYS	B	367	42.524	47.386	44.066	1.00	105.18
	1866	N	GLY	B	368	46.839	52.909	40.422	1.00	98.70
	1867	CA	GLY	B	368	48.136	53.408	40.828	1.00	95.62
	1868	C	GLY	B	368	47.700	54.801	41.244	1.00	93.12
	1869	O	GLY	B	368	46.538	55.143	41.035	1.00	93.17
	1870	N	THR	B	369	48.569	55.617	41.823	1.00	90.15
	1871	CA	THR	B	369	48.125	56.948	42.220	1.00	86.41
	1872	C	THR	B	369	48.420	57.977	41.136	1.00	83.04
	1873	O	THR	B	369	49.402	57.854	40.401	1.00	82.54
	1874	CB	THR	B	369	48.792	57.397	43.541	1.00	87.73
	1875	OG1	THR	B	369	50.217	57.422	43.379	1.00	88.60
	1876	CG2	THR	B	369	48.423	56.443	44.671	1.00	86.64
	1877	N	VAL	B	370	47.552	58.980	41.027	1.00	79.07
	1878	CA	VAL	B	370	47.729	60.041	40.042	1.00	74.46
	1879	C	VAL	B	370	48.275	61.261	40.768	1.00	72.21
	1880	O	VAL	B	370	47.602	61.838	41.618	1.00	71.35
	1881	CB	VAL	B	370	46.401	60.420	39.368	1.00	73.33
	1882	CG1	VAL	B	370	46.667	61.346	38.196	1.00	70.92
	1883	CG2	VAL	B	370	45.674	59.173	38.915	1.00	69.77
	1884	N	ASN	B	371	49.498	61.653	40.426	1.00	70.13
	1885	CA	ASN	B	371	50.137	62.791	41.073	1.00	68.15
	1886	C	ASN	B	371	50.157	64.079	40.262	1.00	65.65
	1887	O	ASN	B	371	50.352	64.067	39.046	1.00	64.64
	1888	CB	ASN	B	371	51.564	62.421	41.469	1.00	70.12
	1889	CG	ASN	B	371	51.605	61.330	42.508	1.00	73.56
	1890	OD1	ASN	B	371	51.153	61.519	43.638	1.00	75.10
	1891	ND2	ASN	B	371	52.137	60.173	42.131	1.00	74.76
	1892	N	LEU	B	372	49.949	65.192	40.959	1.00	62.66
	1893	CA	LEU	B	372	49.959	66.512	40.346	1.00	59.53
	1894	C	LEU	B	372	50.927	67.374	41.137	1.00	56.68
	1895	O	LEU	B	372	50.788	67.529	42.347	1.00	56.70
	1896	CB	LEU	B	372	48.560	67.141	40.372	1.00	59.44
	1897	CG	LEU	B	372	47.428	66.383	39.678	1.00	60.55

	1898	CD1	LEU	B	372	46.214	67.277	39.579	1.00	61.28
	1899	CD2	LEU	B	372	47.861	65.956	38.293	1.00	62.83
	1900	N	THR	B	373	51.911	67.931	40.446	1.00	53.76
	1901	CA	THR	B	373	52.915	68.766	41.085	1.00	51.64
	1902	C	THR	B	373	52.850	70.180	40.512	1.00	48.20
	1903	O	THR	B	373	52.801	70.355	39.296	1.00	46.65
	1904	CB	THR	B	373	54.325	68.201	40.832	1.00	53.15
	1905	OG1	THR	B	373	54.324	66.789	41.073	1.00	57.77
	1906	CG2	THR	B	373	55.339	68.871	41.747	1.00	53.75
	1907	N	TRP	B	374	52.851	71.181	41.385	1.00	45.34
	1908	CA	TRP	B	374	52.799	72.575	40.942	1.00	44.94
	1909	C	TRP	B	374	54.161	73.259	41.041	1.00	43.68
	1910	O	TRP	B	374	54.945	72.964	41.938	1.00	42.67
	1911	CB	TRP	B	374	51.805	73.391	41.784	1.00	41.63
	1912	CG	TRP	B	374	50.371	72.977	41.657	1.00	41.50
	1913	CD1	TRP	B	374	49.688	72.124	42.477	1.00	39.67
	1914	CD2	TRP	B	374	49.441	73.395	40.648	1.00	35.69
	1915	NE1	TRP	B	374	48.392	71.988	42.041	1.00	35.06
	1916	CE2	TRP	B	374	48.214	72.756	40.922	1.00	34.53
	1917	CE3	TRP	B	374	49.528	74.247	39.542	1.00	32.37
	1918	CZ2	TRP	B	374	47.079	72.943	40.129	1.00	35.43
	1919	CZ3	TRP	B	374	48.401	74.434	38.751	1.00	36.11
	1920	CH2	TRP	B	374	47.190	73.782	39.050	1.00	37.51
	1921	N	SER	B	375	54.430	74.179	40.119	1.00	43.53
	1922	CA	SER	B	375	55.678	74.934	40.140	1.00	43.57
	1923	C	SER	B	375	55.511	76.270	39.438	1.00	42.59
	1924	O	SER	B	375	54.669	76.411	38.550	1.00	43.68
	1925	CB	SER	B	375	56.820	74.153	39.474	1.00	45.03
	1926	OG	SER	B	375	56.691	74.118	38.066	1.00	45.66
	1927	N	ARG	B	376	56.299	77.251	39.866	1.00	40.79
	1928	CA	ARG	B	376	56.279	78.569	39.266	1.00	40.12
	1929	C	ARG	B	376	57.498	78.689	38.351	1.00	40.59
	1930	O	ARG	B	376	58.618	78.393	38.752	1.00	40.90
	1931	CB	ARG	B	376	56.345	79.653	40.334	1.00	40.03
	1932	CG	ARG	B	376	55.132	79.745	41.237	1.00	43.20
	1933	CD	ARG	B	376	54.883	81.198	41.599	1.00	41.05
	1934	NE	ARG	B	376	55.171	81.480	42.992	1.00	50.71
	1935	CZ	ARG	B	376	55.300	82.705	43.488	1.00	53.97
	1936	NH1	ARG	B	376	55.172	83.758	42.693	1.00	51.88
	1937	NH2	ARG	B	376	55.542	82.874	44.782	1.00	55.55
	1938	N	ALA	B	377	57.281	79.129	37.122	1.00	40.20
	1939	CA	ALA	B	377	58.382	79.273	36.181	1.00	40.25
	1940	C	ALA	B	377	59.500	80.130	36.786	1.00	40.38
	1941	O	ALA	B	377	60.657	79.979	36.422	1.00	41.16
	1942	CB	ALA	B	377	57.879	79.903	34.878	1.00	33.12
	1943	N	SER	B	378	59.144	81.015	37.714	1.00	40.21
	1944	CA	SER	B	378	60.109	81.903	38.354	1.00	41.95
	1945	C	SER	B	378	60.906	81.188	39.436	1.00	44.92
	1946	O	SER	B	378	61.866	81.744	39.966	1.00	44.28
	1947	CB	SER	B	378	59.401	83.096	38.992	1.00	40.91
	1948	OG	SER	B	378	58.737	82.693	40.180	1.00	40.09
	1949	N	GLY	B	379	60.493	79.967	39.768	1.00	46.93
	1950	CA	GLY	B	379	61.181	79.195	40.787	1.00	49.77
	1951	C	GLY	B	379	60.716	79.512	42.196	1.00	50.60
	1952	O	GLY	B	379	61.024	78.783	43.142	1.00	52.95
	1953	N	LYS	B	380	59.974	80.605	42.345	1.00	53.72
	1954	CA	LYS	B	380	59.478	80.988	43.657	1.00	54.13
	1955	C	LYS	B	380	58.564	79.911	44.255	1.00	48.16
	1956	O	LYS	B	380	58.087	79.008	43.556	1.00	45.65
	1957	CB	LYS	B	380	58.752	82.338	43.583	1.00	62.44
	1958	CG	LYS	B	380	59.692	83.522	43.390	1.00	67.72
	1959	CD	LYS	B	380	58.975	84.852	43.550	1.00	69.32

	1960	CE	LYS	B	380	59.956	86.013	43.481	1.00	73.14
	1961	NZ	LYS	B	380	59.280	87.333	43.633	1.00	77.37
	1962	N	PRO	B	381	58.323	79.986	45.571	1.00	56.07
	1963	CA	PRO	B	381	57.472	79.014	46.265	1.00	56.46
	1964	C	PRO	B	381	55.993	79.065	45.875	1.00	54.32
	1965	O	PRO	B	381	55.446	80.133	45.589	1.00	56.76
	1966	CB	PRO	B	381	57.664	79.375	47.740	1.00	60.70
	1967	CG	PRO	B	381	58.978	80.119	47.767	1.00	62.01
	1968	CD	PRO	B	381	58.905	80.945	46.526	1.00	59.24
	1969	N	VAL	B	382	55.356	77.899	45.866	1.00	55.74
	1970	CA	VAL	B	382	53.931	77.805	45.569	1.00	55.58
	1971	C	VAL	B	382	53.247	77.408	46.880	1.00	55.56
	1972	O	VAL	B	382	53.848	76.734	47.720	1.00	55.22
	1973	CB	VAL	B	382	53.620	76.726	44.493	1.00	55.39
	1974	CG1	VAL	B	382	54.404	77.008	43.222	1.00	55.94
	1975	CG2	VAL	B	382	53.936	75.339	45.025	1.00	53.06
	1976	N	ASN	B	383	52.000	77.827	47.055	1.00	54.38
	1977	CA	ASN	B	383	51.246	77.510	48.264	1.00	54.63
	1978	C	ASN	B	383	50.757	76.068	48.290	1.00	53.85
	1979	O	ASN	B	383	50.970	75.297	47.354	1.00	52.58
	1980	CB	ASN	B	383	50.034	78.429	48.382	1.00	59.07
	1981	CG	ASN	B	383	50.414	79.883	48.456	1.00	64.60
	1982	OD1	ASN	B	383	49.576	80.764	48.269	1.00	70.14
	1983	ND2	ASN	B	383	51.685	80.150	48.738	1.00	71.07
	1984	N	HIS	B	384	50.094	75.710	49.381	1.00	53.46
	1985	CA	HIS	B	384	49.543	74.371	49.526	1.00	52.22
	1986	C	HIS	B	384	48.298	74.274	48.640	1.00	49.10
	1987	O	HIS	B	384	47.495	75.200	48.585	1.00	45.53
	1988	CB	HIS	B	384	49.183	74.111	50.993	1.00	59.11
	1989	CG	HIS	B	384	50.377	73.924	51.878	1.00	62.16
	1990	ND1	HIS	B	384	51.243	72.862	51.739	1.00	69.15
	1991	CD2	HIS	B	384	50.855	74.669	52.903	1.00	70.28
	1992	CE1	HIS	B	384	52.206	72.960	52.639	1.00	75.01
	1993	NE2	HIS	B	384	51.995	74.047	53.358	1.00	74.58
	1994	N	SER	B	385	48.146	73.152	47.949	1.00	45.07
	1995	CA	SER	B	385	47.017	72.959	47.060	1.00	44.61
	1996	C	SER	B	385	45.973	71.983	47.604	1.00	44.58
	1997	O	SER	B	385	46.244	71.220	48.521	1.00	44.21
	1998	CB	SER	B	385	47.524	72.487	45.691	1.00	44.61
	1999	OG	SER	B	385	48.310	71.307	45.789	1.00	41.13
	2000	N	THR	B	386	44.773	72.025	47.035	1.00	44.32
	2001	CA	THR	B	386	43.684	71.150	47.446	1.00	44.35
	2002	C	THR	B	386	43.444	70.113	46.363	1.00	44.09
	2003	O	THR	B	386	43.274	70.451	45.189	1.00	44.06
	2004	CB	THR	B	386	42.374	71.936	47.680	1.00	45.20
	2005	OG1	THR	B	386	42.555	72.856	48.762	1.00	51.89
	2006	CG2	THR	B	386	41.232	70.984	48.036	1.00	47.20
	2007	N	ARG	B	387	43.424	68.851	46.774	1.00	44.39
	2008	CA	ARG	B	387	43.222	67.730	45.867	1.00	46.68
	2009	C	ARG	B	387	41.837	67.080	46.030	1.00	47.05
	2010	O	ARG	B	387	41.372	66.850	47.149	1.00	46.65
	2011	CB	ARG	B	387	44.316	66.694	46.121	1.00	48.13
	2012	CG	ARG	B	387	44.270	65.488	45.210	1.00	52.77
	2013	CD	ARG	B	387	45.106	64.353	45.780	1.00	56.60
	2014	NE	ARG	B	387	44.978	63.141	44.979	1.00	60.65
	2015	CZ	ARG	B	387	45.683	62.895	43.882	1.00	61.97
	2016	NH1	ARG	B	387	46.578	63.779	43.464	1.00	64.45
	2017	NH2	ARG	B	387	45.469	61.781	43.189	1.00	60.54
	2018	N	LYS	B	388	41.185	66.780	44.910	1.00	46.93
	2019	CA	LYS	B	388	39.870	66.143	44.933	1.00	47.51
	2020	C	LYS	B	388	39.823	64.970	43.957	1.00	48.33
	2021	O	LYS	B	388	40.199	65.107	42.794	1.00	46.08

	2022	CB	LYS	B	388	38.777	67.148	44.563	1.00	46.64
	2023	CG	LYS	B	388	38.691	68.326	45.497	1.00	52.75
	2024	CD	LYS	B	388	37.861	69.446	44.905	1.00	58.62
	2025	CE	LYS	B	388	38.062	70.737	45.682	1.00	62.49
	2026	NZ	LYS	B	388	37.396	71.881	44.999	1.00	67.33
	2027	N	GLU	B	389	39.364	63.820	44.449	1.00	50.07
	2028	CA	GLU	B	389	39.243	62.602	43.646	1.00	51.86
	2029	C	GLU	B	389	37.793	62.126	43.638	1.00	52.81
	2030	O	GLU	B	389	37.192	61.917	44.695	1.00	49.21
	2031	CB	GLU	B	389	40.126	61.494	44.223	1.00	54.67
	2032	CG	GLU	B	389	41.616	61.710	44.044	1.00	65.65
	2033	CD	GLU	B	389	42.441	60.608	44.688	1.00	72.66
	2034	OE1	GLU	B	389	42.151	59.418	44.429	1.00	75.92
	2035	OE2	GLU	B	389	43.380	60.931	45.450	1.00	75.78
	2036	N	GLU	B	390	37.229	61.948	42.449	1.00	56.06
	2037	CA	GLU	B	390	35.849	61.500	42.346	1.00	61.17
	2038	C	GLU	B	390	35.629	60.454	41.265	1.00	64.70
	2039	O	GLU	B	390	36.072	60.598	40.123	1.00	64.01
	2040	CB	GLU	B	390	34.927	62.692	42.107	1.00	64.35
	2041	CG	GLU	B	390	33.479	62.317	41.867	1.00	74.80
	2042	CD	GLU	B	390	32.548	63.509	41.979	1.00	85.97
	2043	OE1	GLU	B	390	32.822	64.547	41.336	1.00	92.60
	2044	OE2	GLU	B	390	31.541	63.403	42.712	1.00	92.18
	2045	N	LYS	B	391	34.921	59.396	41.639	1.00	68.18
	2046	CA	LYS	B	391	34.640	58.312	40.712	1.00	71.58
	2047	C	LYS	B	391	33.215	58.302	40.180	1.00	76.11
	2048	O	LYS	B	391	32.265	58.673	40.869	1.00	75.89
	2049	CB	LYS	B	391	34.946	56.973	41.372	1.00	67.28
	2050	N	GLN	B	392	33.092	57.876	38.932	1.00	81.85
	2051	CA	GLN	B	392	31.814	57.746	38.254	1.00	88.38
	2052	C	GLN	B	392	32.026	56.482	37.443	1.00	92.30
	2053	O	GLN	B	392	32.752	56.500	36.452	1.00	93.25
	2054	CB	GLN	B	392	31.555	58.938	37.323	1.00	85.87
	2055	CG	GLN	B	392	30.422	59.848	37.782	1.00	90.76
	2056	CD	GLN	B	392	30.027	60.873	36.731	1.00	93.39
	2057	OE1	GLN	B	392	29.687	60.524	35.598	1.00	92.93
	2058	NE2	GLN	B	392	30.062	62.147	37.107	1.00	93.97
	2059	N	ARG	B	393	31.426	55.379	37.880	1.00	96.24
	2060	CA	ARG	B	393	31.589	54.108	37.184	1.00	100.53
	2061	C	ARG	B	393	31.250	54.188	35.697	1.00	102.30
	2062	O	ARG	B	393	31.273	53.178	34.993	1.00	101.15
	2063	CB	ARG	B	393	30.747	53.021	37.855	1.00	106.99
	2064	CG	ARG	B	393	29.251	53.196	37.704	1.00	109.77
	2065	CD	ARG	B	393	28.521	52.107	38.464	1.00	115.73
	2066	NE	ARG	B	393	27.095	52.085	38.165	1.00	119.73
	2067	CZ	ARG	B	393	26.227	51.267	38.750	1.00	121.60
	2068	NH1	ARG	B	393	26.645	50.406	39.670	1.00	121.59
	2069	NH2	ARG	B	393	24.945	51.308	38.416	1.00	121.49
	2070	N	ASN	B	394	30.942	55.391	35.224	1.00	103.98
	2071	CA	ASN	B	394	30.630	55.595	33.819	1.00	106.60
	2072	C	ASN	B	394	31.918	55.325	33.049	1.00	106.89
	2073	O	ASN	B	394	31.950	54.516	32.122	1.00	108.55
	2074	CB	ASN	B	394	30.173	57.036	33.580	1.00	106.97
	2075	CG	ASN	B	394	29.709	57.274	32.153	1.00	112.83
	2076	OD1	ASN	B	394	29.459	58.410	31.752	1.00	114.53
	2077	ND2	ASN	B	394	29.584	56.198	31.381	1.00	114.40
	2078	N	GLY	B	395	32.984	56.007	33.452	1.00	105.53
	2079	CA	GLY	B	395	34.269	55.829	32.802	1.00	101.15
	2080	C	GLY	B	395	35.177	57.015	33.050	1.00	97.82
	2081	O	GLY	B	395	35.879	57.475	32.148	1.00	99.41
	2082	N	THR	B	396	35.177	57.516	34.278	1.00	94.50
	2083	CA	THR	B	396	36.011	58.663	34.578	1.00	89.02

	2084	C	THR	B	396	36.426	58.837	36.029	1.00	83.93
	2085	O	THR	B	396	35.600	59.123	36.896	1.00	83.27
	2086	CB	THR	B	396	35.322	59.975	34.130	1.00	92.03
	2087	OG1	THR	B	396	35.116	59.952	32.712	1.00	94.17
	2088	CG2	THR	B	396	36.179	61.186	34.504	1.00	95.48
	2089	N	LEU	B	397	37.718	58.658	36.279	1.00	79.69
	2090	CA	LEU	B	397	38.280	58.871	37.600	1.00	74.75
	2091	C	LEU	B	397	38.773	60.305	37.496	1.00	71.50
	2092	O	LEU	B	397	39.880	60.548	37.019	1.00	74.81
	2093	CB	LEU	B	397	39.480	57.960	37.860	1.00	75.72
	2094	CG	LEU	B	397	40.350	58.412	39.047	1.00	70.67
	2095	CD1	LEU	B	397	39.742	57.932	40.362	1.00	69.05
	2096	CD2	LEU	B	397	41.768	57.877	38.887	1.00	72.96
	2097	N	THR	B	398	37.941	61.252	37.905	1.00	67.61
	2098	CA	THR	B	398	38.314	62.655	37.848	1.00	61.30
	2099	C	THR	B	398	39.207	63.041	39.024	1.00	56.61
	2100	O	THR	B	398	38.974	62.640	40.166	1.00	54.95
	2101	CB	THR	B	398	37.070	63.556	37.852	1.00	61.75
	2102	OG1	THR	B	398	36.345	63.375	36.629	1.00	65.40
	2103	CG2	THR	B	398	37.471	65.016	37.992	1.00	63.39
	2104	N	VAL	B	399	40.241	63.817	38.729	1.00	51.84
	2105	CA	VAL	B	399	41.163	64.279	39.751	1.00	48.05
	2106	C	VAL	B	399	41.515	65.730	39.490	1.00	44.81
	2107	O	VAL	B	399	41.911	66.098	38.381	1.00	44.41
	2108	CB	VAL	B	399	42.466	63.468	39.751	1.00	49.35
	2109	CG1	VAL	B	399	43.409	64.010	40.805	1.00	49.43
	2110	CG2	VAL	B	399	42.168	62.006	40.010	1.00	53.10
	2111	N	THR	B	400	41.354	66.564	40.504	1.00	42.44
	2112	CA	THR	B	400	41.691	67.965	40.343	1.00	40.44
	2113	C	THR	B	400	42.532	68.449	41.498	1.00	38.07
	2114	O	THR	B	400	42.483	67.908	42.602	1.00	36.13
	2115	CB	THR	B	400	40.448	68.869	40.266	1.00	39.64
	2116	OG1	THR	B	400	39.845	68.962	41.561	1.00	43.72
	2117	CG2	THR	B	400	39.442	68.322	39.278	1.00	38.32
	2118	N	SER	B	401	43.335	69.460	41.216	1.00	36.90
	2119	CA	SER	B	401	44.168	70.069	42.224	1.00	35.46
	2120	C	SER	B	401	43.988	71.557	42.016	1.00	33.95
	2121	O	SER	B	401	44.153	72.062	40.908	1.00	34.80
	2122	CB	SER	B	401	45.638	69.694	42.040	1.00	36.91
	2123	OG	SER	B	401	46.417	70.301	43.060	1.00	40.84
	2124	N	THR	B	402	43.635	72.248	43.086	1.00	32.28
	2125	CA	THR	B	402	43.422	73.672	43.032	1.00	31.85
	2126	C	THR	B	402	44.508	74.355	43.836	1.00	31.76
	2127	O	THR	B	402	44.737	74.046	45.010	1.00	30.55
	2128	CB	THR	B	402	42.051	74.030	43.595	1.00	31.33
	2129	OG1	THR	B	402	41.058	73.316	42.862	1.00	32.83
	2130	CG2	THR	B	402	41.782	75.522	43.468	1.00	32.70
	2131	N	LEU	B	403	45.167	75.301	43.188	1.00	30.72
	2132	CA	LEU	B	403	46.257	76.018	43.800	1.00	30.33
	2133	C	LEU	B	403	45.927	77.485	44.003	1.00	29.66
	2134	O	LEU	B	403	45.608	78.185	43.048	1.00	28.06
	2135	CB	LEU	B	403	47.502	75.902	42.913	1.00	28.34
	2136	CG	LEU	B	403	48.769	76.632	43.381	1.00	32.10
	2137	CD1	LEU	B	403	49.425	75.823	44.503	1.00	31.94
	2138	CD2	LEU	B	403	49.756	76.790	42.224	1.00	30.42
	2139	N	PRO	B	404	45.983	77.962	45.259	1.00	31.48
	2140	CA	PRO	B	404	45.704	79.367	45.566	1.00	33.20
	2141	C	PRO	B	404	46.841	80.149	44.906	1.00	34.02
	2142	O	PRO	B	404	47.999	79.755	44.996	1.00	32.25

	2143	CB	PRO	B	404	45.788	79.417	47.090	1.00	33.28
	2144	CG	PRO	B	404	45.435	78.010	47.500	1.00	31.82
	2145	CD	PRO	B	404	46.186	77.187	46.497	1.00	31.26
	2146	N	VAL	B	405	46.503	81.238	44.235	1.00	34.94
5	2147	CA	VAL	B	405	47.483	82.044	43.536	1.00	38.63
	2148	C	VAL	B	405	47.541	83.472	44.068	1.00	40.02
	2149	O	VAL	B	405	46.537	84.027	44.502	1.00	40.31
	2150	CB	VAL	B	405	47.143	82.052	42.018	1.00	42.09
	2151	CG1	VAL	B	405	47.110	83.472	41.468	1.00	43.95
10	2152	CG2	VAL	B	405	48.144	81.195	41.273	1.00	41.76
	2153	N	GLY	B	406	48.728	84.064	44.039	1.00	42.35
	2154	CA	GLY	B	406	48.859	85.432	44.503	1.00	43.35
	2155	C	GLY	B	406	48.178	86.354	43.513	1.00	43.87
	2156	O	GLY	B	406	48.286	86.154	42.303	1.00	42.68
15	2157	N	THR	B	407	47.466	87.352	44.023	1.00	44.40
	2158	CA	THR	B	407	46.760	88.306	43.177	1.00	47.37
	2159	C	THR	B	407	47.713	89.127	42.322	1.00	48.27
	2160	O	THR	B	407	47.549	89.208	41.107	1.00	48.77
	2161	CB	THR	B	407	45.922	89.288	44.022	1.00	48.44
20	2162	OG1	THR	B	407	44.809	88.599	44.596	1.00	50.00
	2163	CG2	THR	B	407	45.413	90.436	43.162	1.00	53.23
	2164	N	ARG	B	408	48.697	89.746	42.970	1.00	48.10
	2165	CA	ARG	B	408	49.665	90.579	42.279	1.00	48.54
	2166	C	ARG	B	408	50.540	89.773	41.335	1.00	48.48
25	2167	O	ARG	B	408	50.769	90.182	40.197	1.00	47.34
	2168	CB	ARG	B	408	50.530	91.325	43.290	1.00	50.16
	2169	N	ASP	B	409	51.033	88.634	41.806	1.00	48.72
	2170	CA	ASP	B	409	51.886	87.787	40.979	1.00	50.88
	2171	C	ASP	B	409	51.187	87.421	39.674	1.00	49.92
30	2172	O	ASP	B	409	51.789	87.468	38.598	1.00	49.76
	2173	CB	ASP	B	409	52.260	86.512	41.738	1.00	56.18
	2174	CG	ASP	B	409	53.013	86.801	43.026	1.00	64.80
	2175	OD1	ASP	B	409	54.062	87.482	42.956	1.00	71.41
	2176	OD2	ASP	B	409	52.561	86.353	44.105	1.00	68.29
35	2177	N	TRP	B	410	49.908	87.067	39.773	1.00	48.36
	2178	CA	TRP	B	410	49.142	86.686	38.597	1.00	46.32
	2179	C	TRP	B	410	48.953	87.864	37.653	1.00	46.21
	2180	O	TRP	B	410	49.111	87.731	36.440	1.00	44.64
	2181	CB	TRP	B	410	47.774	86.120	38.992	1.00	42.82
40	2182	CG	TRP	B	410	47.001	85.710	37.796	1.00	39.31
	2183	CD1	TRP	B	410	46.104	86.467	37.103	1.00	37.29
	2184	CD2	TRP	B	410	47.181	84.507	37.043	1.00	35.49
	2185	NE1	TRP	B	410	45.726	85.819	35.957	1.00	39.24
	2186	CE2	TRP	B	410	46.372	84.613	35.895	1.00	32.76
45	2187	CE3	TRP	B	410	47.956	83.351	37.228	1.00	32.07
	2188	CZ2	TRP	B	410	46.309	83.606	34.924	1.00	29.59
	2189	CZ3	TRP	B	410	47.896	82.352	36.269	1.00	33.68
	2190	CH2	TRP	B	410	47.073	82.489	35.125	1.00	30.56
	2191	N	ILE	B	411	48.611	89.016	38.212	1.00	48.11
50	2192	CA	ILE	B	411	48.408	90.209	37.401	1.00	50.90
	2193	C	ILE	B	411	49.712	90.649	36.742	1.00	52.46
	2194	O	ILE	B	411	49.698	91.229	35.658	1.00	53.34
	2195	CB	ILE	B	411	47.845	91.366	38.246	1.00	51.58
	2196	CG1	ILE	B	411	46.456	90.987	38.770	1.00	52.81
55	2197	CG2	ILE	B	411	47.772	92.634	37.415	1.00	51.95
	2198	CD1	ILE	B	411	45.823	92.034	39.669	1.00	59.38
	2199	N	GLU	B	412	50.837	90.348	37.385	1.00	53.21
	2200	CA	GLU	B	412	52.137	90.728	36.852	1.00	53.12
	2201	C	GLU	B	412	52.681	89.747	35.831	1.00	51.24
5	2202	O	GLU	B	412	53.736	89.990	35.252	1.00	51.40
	2203	CB	GLU	B	412	53.152	90.909	37.981	1.00	59.71

	2204	CG	GLU	B	412	53.022	92.238	38.717	1.00	70.52
	2205	CD	GLU	B	412	54.060	92.399	39.810	1.00	78.58
	2206	OE1	GLU	B	412	55.262	92.198	39.527	1.00	83.44
	2207	OE2	GLU	B	412	53.676	92.732	40.950	1.00	82.10
	2208	N	GLY	B	413	51.982	88.634	35.623	1.00	48.47
	2209	CA	GLY	B	413	52.427	87.677	34.626	1.00	44.62
	2210	C	GLY	B	413	53.116	86.387	35.032	1.00	44.15
	2211	O	GLY	B	413	53.687	85.718	34.173	1.00	43.50
	2212	N	GLU	B	414	53.085	86.012	36.307	1.00	42.78
	2213	CA	GLU	B	414	53.722	84.757	36.694	1.00	40.78
	2214	C	GLU	B	414	53.105	83.652	35.851	1.00	39.97
	2215	O	GLU	B	414	51.955	83.758	35.410	1.00	37.43
	2216	CB	GLU	B	414	53.489	84.445	38.182	1.00	41.96
	2217	CG	GLU	B	414	54.034	83.081	38.659	1.00	44.09
	2218	CD	GLU	B	414	55.564	83.018	38.740	1.00	49.01
	2219	OE1	GLU	B	414	56.213	82.549	37.775	1.00	46.84
	2220	OE2	GLU	B	414	56.121	83.448	39.773	1.00	49.89
	2221	N	THR	B	415	53.879	82.599	35.615	1.00	39.56
	2222	CA	THR	B	415	53.403	81.464	34.847	1.00	40.76
	2223	C	THR	B	415	53.487	80.231	35.738	1.00	40.07
	2224	O	THR	B	415	54.533	79.960	36.323	1.00	42.10
	2225	CB	THR	B	415	54.238	81.273	33.556	1.00	44.69
	2226	OG1	THR	B	415	54.222	79.893	33.171	1.00	51.98
	2227	CG2	THR	B	415	55.652	81.744	33.758	1.00	50.00
	2228	N	TYR	B	416	52.380	79.500	35.860	1.00	37.57
	2229	CA	TYR	B	416	52.327	78.318	36.714	1.00	34.50
	2230	C	TYR	B	416	52.265	77.051	35.899	1.00	36.77
	2231	O	TYR	B	416	51.706	77.038	34.800	1.00	35.94
	2232	CB	TYR	B	416	51.116	78.379	37.634	1.00	34.15
	2233	CG	TYR	B	416	51.085	79.597	38.514	1.00	30.65
	2234	CD1	TYR	B	416	50.777	80.856	37.992	1.00	32.53
	2235	CD2	TYR	B	416	51.389	79.499	39.865	1.00	31.72
	2236	CE1	TYR	B	416	50.772	81.984	38.803	1.00	34.27
	2237	CE2	TYR	B	416	51.390	80.619	40.680	1.00	32.11
	2238	CZ	TYR	B	416	51.080	81.856	40.144	1.00	33.86
	2239	OH	TYR	B	416	51.082	82.964	40.961	1.00	41.22
	2240	N	GLN	B	417	52.829	75.976	36.441	1.00	37.58
	2241	CA	GLN	B	417	52.848	74.722	35.714	1.00	39.43
	2242	C	GLN	B	417	52.341	73.538	36.518	1.00	39.40
	2243	O	GLN	B	417	52.664	73.373	37.694	1.00	39.63
	2244	CB	GLN	B	417	54.269	74.421	35.211	1.00	41.37
	2245	CG	GLN	B	417	54.350	73.214	34.278	1.00	51.81
	2246	CD	GLN	B	417	55.773	72.856	33.886	1.00	61.69
	2247	OE1	GLN	B	417	56.555	72.371	34.710	1.00	67.15
	2248	NE2	GLN	B	417	56.119	73.096	32.621	1.00	63.64
	2249	N	CYS	B	418	51.543	72.712	35.864	1.00	39.29
	2250	CA	CYS	B	418	51.019	71.517	36.489	1.00	41.80
	2251	C	CYS	B	418	51.720	70.350	35.818	1.00	42.50
	2252	O	CYS	B	418	51.646	70.191	34.600	1.00	43.33
	2253	CB	CYS	B	418	49.501	71.392	36.275	1.00	41.95
	2254	SG	CYS	B	418	48.795	69.904	37.057	1.00	54.15
	2255	N	ARG	B	419	52.418	69.551	36.609	1.00	43.98
	2256	CA	ARG	B	419	53.103	68.375	36.093	1.00	47.51
	2257	C	ARG	B	419	52.277	67.172	36.542	1.00	48.11
	2258	O	ARG	B	419	52.219	66.859	37.730	1.00	47.85
	2259	CB	ARG	B	419	54.532	68.311	36.648	1.00	49.08
	2260	CG	ARG	B	419	55.203	66.958	36.514	1.00	54.11
	2261	CD	ARG	B	419	56.708	67.046	36.796	1.00	64.71
	2262	NE	ARG	B	419	57.325	65.732	36.963	1.00	64.09
	2263	CZ	ARG	B	419	57.437	65.107	38.132	1.00	70.31
	2264	NH1	ARG	B	419	56.981	65.681	39.239	1.00	68.32
	2265	NH2	ARG	B	419	57.992	63.901	38.195	1.00	71.53

	2266	N	VAL	B	420	51.610	66.524	35.592	1.00	51.04
	2267	CA	VAL	B	420	50.776	65.369	35.900	1.00	56.22
	2268	C	VAL	B	420	51.561	64.068	35.746	1.00	61.25
	2269	O	VAL	B	420	52.178	63.820	34.707	1.00	60.11
	2270	CB	VAL	B	420	49.536	65.305	34.985	1.00	54.44
	2271	CG1	VAL	B	420	48.678	64.106	35.371	1.00	52.69
	2272	CG2	VAL	B	420	48.732	66.597	35.095	1.00	55.45
	2273	N	THR	B	421	51.529	63.241	36.786	1.00	66.23
	2274	CA	THR	B	421	52.244	61.969	36.774	1.00	73.18
	2275	C	THR	B	421	51.334	60.766	36.970	1.00	76.87
	2276	O	THR	B	421	50.968	60.443	38.100	1.00	77.93
	2277	CB	THR	B	421	53.317	61.929	37.875	1.00	73.75
	2278	OG1	THR	B	421	54.272	62.972	37.649	1.00	77.71
	2279	CG2	THR	B	421	54.033	60.591	37.873	1.00	75.35
	2280	N	HIS	B	422	50.976	60.101	35.874	1.00	81.02
	2281	CA	HIS	B	422	50.117	58.922	35.949	1.00	86.07
	2282	C	HIS	B	422	51.004	57.686	35.822	1.00	89.67
	2283	O	HIS	B	422	51.920	57.653	35.002	1.00	90.00
	2284	CB	HIS	B	422	49.071	58.940	34.831	1.00	87.43
	2285	CG	HIS	B	422	47.892	58.052	35.092	1.00	90.73
	2286	ND1	HIS	B	422	47.076	58.203	36.191	1.00	93.83
	2287	CD2	HIS	B	422	47.396	57.000	34.396	1.00	91.89
	2288	CE1	HIS	B	422	46.127	57.282	36.164	1.00	94.70
	2289	NE2	HIS	B	422	46.300	56.540	35.085	1.00	93.25
	2290	N	PRO	B	423	50.729	56.646	36.626	1.00	92.64
	2291	CA	PRO	B	423	51.489	55.391	36.640	1.00	95.19
	2292	C	PRO	B	423	51.972	54.762	35.325	1.00	97.06
	2293	O	PRO	B	423	53.169	54.536	35.155	1.00	97.57
	2294	CB	PRO	B	423	50.576	54.445	37.433	1.00	95.56
	2295	CG	PRO	B	423	49.209	55.034	37.247	1.00	93.94
	2296	CD	PRO	B	423	49.488	56.495	37.404	1.00	93.12
	2297	N	HIS	B	424	51.058	54.495	34.399	1.00	98.71
	2298	CA	HIS	B	424	51.410	53.831	33.143	1.00	100.16
	2299	C	HIS	B	424	52.104	54.579	32.005	1.00	99.67
	2300	O	HIS	B	424	52.910	53.991	31.284	1.00	99.61
	2301	CB	HIS	B	424	50.165	53.149	32.578	1.00	102.42
	2302	CG	HIS	B	424	49.578	52.125	33.495	1.00	105.47
	2303	ND1	HIS	B	424	48.302	52.228	34.008	1.00	107.10
	2304	CD2	HIS	B	424	50.079	50.961	33.967	1.00	97.46
	2305	CE1	HIS	B	424	48.044	51.170	34.755	1.00	106.81
	2306	NE2	HIS	B	424	49.106	50.385	34.747	1.00	106.61
	2307	N	LEU	B	425	51.802	55.858	31.833	1.00	99.19
	2308	CA	LEU	B	425	52.384	56.628	30.737	1.00	99.01
	2309	C	LEU	B	425	53.886	56.908	30.816	1.00	98.36
	2310	O	LEU	B	425	54.440	57.121	31.896	1.00	98.39
	2311	CB	LEU	B	425	51.606	57.929	30.593	1.00	100.66
	2312	CG	LEU	B	425	50.105	57.631	30.633	1.00	101.95
	2313	CD1	LEU	B	425	49.315	58.917	30.531	1.00	102.59
	2314	CD2	LEU	B	425	49.744	56.677	29.502	1.00	103.85
	2315	N	PRO	B	426	54.562	56.915	29.652	1.00	97.57
	2316	CA	PRO	B	426	56.004	57.165	29.560	1.00	96.82
	2317	C	PRO	B	426	56.414	58.525	30.108	1.00	95.53
	2318	O	PRO	B	426	57.040	58.610	31.163	1.00	95.77
	2319	CB	PRO	B	426	56.282	57.030	28.063	1.00	97.13
	2320	CG	PRO	B	426	54.995	57.494	27.440	1.00	97.88
	2321	CD	PRO	B	426	53.969	56.798	28.307	1.00	97.70
	2322	N	ARG	B	427	56.064	59.585	29.387	1.00	94.16
	2323	CA	ARG	B	427	56.402	60.931	29.826	1.00	92.52
	2324	C	ARG	B	427	55.285	61.509	30.692	1.00	89.85
	2325	O	ARG	B	427	54.123	61.113	30.583	1.00	89.26
	2326	CB	ARG	B	427	56.652	61.851	28.622	1.00	97.34
	2327	CG	ARG	B	427	57.202	63.219	29.023	1.00	99.32

	2328	CD	ARG	B	427	57.407	64.172	27.847	1.00	105.99
	2329	NE	ARG	B	427	58.068	65.403	28.285	1.00	111.10
	2330	CZ	ARG	B	427	58.302	66.460	27.512	1.00	111.66
	2331	NH1	ARG	B	427	57.927	66.457	26.239	1.00	111.70
	2332	NH2	ARG	B	427	58.921	67.522	28.013	1.00	110.09
	2333	N	ALA	B	428	55.651	62.442	31.562	1.00	86.56
	2334	CA	ALA	B	428	54.690	63.087	32.439	1.00	82.70
	2335	C	ALA	B	428	53.998	64.211	31.677	1.00	80.03
	2336	O	ALA	B	428	54.619	64.889	30.861	1.00	80.29
	2337	CB	ALA	B	428	55.400	63.647	33.663	1.00	83.85
	2338	N	LEU	B	429	52.708	64.397	31.936	1.00	76.76
	2339	CA	LEU	B	429	51.949	65.456	31.285	1.00	72.72
	2340	C	LEU	B	429	52.311	66.780	31.936	1.00	69.67
	2341	O	LEU	B	429	52.472	66.858	33.153	1.00	68.64
	2342	CB	LEU	B	429	50.444	65.208	31.429	1.00	73.60
	2343	CG	LEU	B	429	49.753	64.431	30.307	1.00	73.35
	2344	CD1	LEU	B	429	48.320	64.102	30.696	1.00	72.09
	2345	CD2	LEU	B	429	49.787	65.267	29.035	1.00	76.40
	2346	N	MET	B	430	52.447	67.821	31.124	1.00	66.83
	2347	CA	MET	B	430	52.786	69.132	31.651	1.00	64.81
	2348	C	MET	B	430	51.922	70.216	31.026	1.00	61.41
	2349	O	MET	B	430	51.824	70.326	29.801	1.00	60.84
	2350	CB	MET	B	430	54.265	69.427	31.409	1.00	68.22
	2351	CG	MET	B	430	55.184	68.353	31.967	1.00	74.39
	2352	SD	MET	B	430	56.921	68.714	31.713	1.00	83.18
	2353	CE	MET	B	430	56.993	68.764	29.906	1.00	84.12
	2354	N	ARG	B	431	51.288	71.010	31.882	1.00	57.17
	2355	CA	ARG	B	431	50.428	72.094	31.426	1.00	54.04
	2356	C	ARG	B	431	50.848	73.366	32.137	1.00	50.58
	2357	O	ARG	B	431	51.233	73.330	33.304	1.00	50.46
	2358	CB	ARG	B	431	48.959	71.775	31.736	1.00	55.16
	2359	CG	ARG	B	431	48.413	70.564	30.991	1.00	59.24
	2360	CD	ARG	B	431	48.428	70.798	29.489	1.00	63.93
	2361	NE	ARG	B	431	48.014	69.617	28.737	1.00	70.30
	2362	CZ	ARG	B	431	48.043	69.530	27.411	1.00	76.24
	2363	NH1	ARG	B	431	48.469	70.559	26.683	1.00	77.83
	2364	NH2	ARG	B	431	47.648	68.415	26.811	1.00	77.12
	2365	N	SER	B	432	50.788	74.488	31.431	1.00	46.92
	2366	CA	SER	B	432	51.163	75.765	32.016	1.00	45.15
	2367	C	SER	B	432	50.118	76.816	31.702	1.00	42.49
	2368	O	SER	B	432	49.382	76.699	30.721	1.00	42.76
	2369	CB	SER	B	432	52.532	76.206	31.490	1.00	44.31
	2370	OG	SER	B	432	52.516	76.284	30.082	1.00	49.96
	2371	N	THR	B	433	50.060	77.851	32.530	1.00	40.28
	2372	CA	THR	B	433	49.078	78.909	32.337	1.00	39.71
	2373	C	THR	B	433	49.604	80.244	32.843	1.00	39.49
	2374	O	THR	B	433	50.414	80.285	33.766	1.00	40.22
	2375	CB	THR	B	433	47.761	78.577	33.078	1.00	38.07
	2376	OG1	THR	B	433	46.793	79.594	32.805	1.00	39.56
	2377	CG2	THR	B	433	47.991	78.512	34.582	1.00	36.99
	2378	N	THR	B	434	49.139	81.328	32.226	1.00	39.18
	2379	CA	THR	B	434	49.532	82.687	32.588	1.00	40.70
	2380	C	THR	B	434	48.414	83.635	32.166	1.00	40.23
	2381	O	THR	B	434	47.509	83.236	31.441	1.00	41.18
	2382	CB	THR	B	434	50.816	83.116	31.844	1.00	43.01
	2383	OG1	THR	B	434	50.548	83.238	30.439	1.00	47.85
	2384	CG2	THR	B	434	51.874	82.076	31.995	1.00	48.67
	2385	N	LYS	B	435	48.475	84.886	32.604	1.00	40.97
	2386	CA	LYS	B	435	47.450	85.833	32.211	1.00	45.73
	2387	C	LYS	B	435	47.579	85.999	30.702	1.00	48.93
	2388	O	LYS	B	435	48.670	85.890	30.158	1.00	48.49
	2389	CB	LYS	B	435	47.663	87.166	32.906	1.00	45.94

	2390	N	THR	B	436	46.467	86.235	30.018	1.00	52.01
	2391	CA	THR	B	436	46.520	86.429	28.574	1.00	54.88
	2392	C	THR	B	436	46.916	87.878	28.326	1.00	55.70
	2393	O	THR	B	436	46.454	88.777	29.023	1.00	55.21
	2394	CB	THR	B	436	45.146	86.162	27.909	1.00	56.24
	2395	OG1	THR	B	436	44.798	84.779	28.062	1.00	60.56
	2396	CG2	THR	B	436	45.188	86.510	26.423	1.00	57.04
	2397	N	SER	B	437	47.790	88.099	27.352	1.00	57.93
	2398	CA	SER	B	437	48.220	89.451	27.020	1.00	60.42
	2399	C	SER	B	437	47.361	89.917	25.851	1.00	60.49
	2400	O	SER	B	437	46.397	89.243	25.477	1.00	60.21
	2401	CB	SER	B	437	49.706	89.467	26.630	1.00	61.57
	2402	OG	SER	B	437	49.949	88.643	25.500	1.00	65.51
	2403	N	GLY	B	438	47.705	91.067	25.279	1.00	60.09
	2404	CA	GLY	B	438	46.934	91.578	24.161	1.00	58.42
	2405	C	GLY	B	438	45.970	92.663	24.589	1.00	57.80
	2406	O	GLY	B	438	45.853	92.952	25.778	1.00	56.51
	2407	N	PRO	B	439	45.267	93.291	23.633	1.00	57.81
	2408	CA	PRO	B	439	44.305	94.358	23.915	1.00	56.19
	2409	C	PRO	B	439	43.178	93.908	24.837	1.00	53.91
	2410	O	PRO	B	439	42.891	92.714	24.953	1.00	53.91
	2411	CB	PRO	B	439	43.794	94.735	22.524	1.00	57.79
	2412	CG	PRO	B	439	44.967	94.453	21.652	1.00	58.60
	2413	CD	PRO	B	439	45.427	93.115	22.179	1.00	60.65
	2414	N	ARG	B	440	42.545	94.878	25.488	1.00	51.09
	2415	CA	ARG	B	440	41.437	94.610	26.398	1.00	48.90
	2416	C	ARG	B	440	40.235	95.380	25.869	1.00	45.83
	2417	O	ARG	B	440	40.398	96.412	25.219	1.00	45.88
	2418	CB	ARG	B	440	41.764	95.099	27.811	1.00	49.95
	2419	CG	ARG	B	440	43.127	94.681	28.329	1.00	59.03
	2420	CD	ARG	B	440	43.227	93.194	28.652	1.00	65.31
	2421	NE	ARG	B	440	44.627	92.786	28.758	1.00	72.31
	2422	CZ	ARG	B	440	45.047	91.614	29.222	1.00	74.99
	2423	NH1	ARG	B	440	44.181	90.706	29.640	1.00	77.22
	2424	NH2	ARG	B	440	46.345	91.348	29.263	1.00	78.59
	2425	N	ALA	B	441	39.036	94.873	26.143	1.00	42.09
	2426	CA	ALA	B	441	37.800	95.521	25.713	1.00	39.26
	2427	C	ALA	B	441	36.706	95.124	26.687	1.00	38.22
	2428	O	ALA	B	441	36.566	93.951	27.024	1.00	38.95
	2429	CB	ALA	B	441	37.430	95.089	24.302	1.00	36.56
	2430	N	ALA	B	442	35.934	96.104	27.134	1.00	37.22
	2431	CA	ALA	B	442	34.871	95.861	28.089	1.00	37.60
	2432	C	ALA	B	442	33.721	95.050	27.520	1.00	38.65
	2433	O	ALA	B	442	33.497	95.047	26.302	1.00	40.22
	2434	CB	ALA	B	442	34.352	97.185	28.629	1.00	37.17
	2435	N	PRO	B	443	32.981	94.340	28.378	1.00	38.04
	2436	CA	PRO	B	443	31.835	93.511	27.996	1.00	36.79
	2437	C	PRO	B	443	30.581	94.376	27.857	1.00	38.14
	2438	O	PRO	B	443	30.426	95.364	28.579	1.00	37.39
	2439	CB	PRO	B	443	31.677	92.550	29.179	1.00	36.30
	2440	CG	PRO	B	443	32.968	92.654	29.941	1.00	36.35
	2441	CD	PRO	B	443	33.351	94.088	29.780	1.00	37.85
	2442	N	GLU	B	444	29.706	94.006	26.927	1.00	36.28
	2443	CA	GLU	B	444	28.437	94.699	26.729	1.00	35.57
	2444	C	GLU	B	444	27.429	93.659	27.212	1.00	33.87
	2445	O	GLU	B	444	27.495	92.490	26.809	1.00	33.43
	2446	CB	GLU	B	444	28.217	95.020	25.249	1.00	38.68
	2447	N	VAL	B	445	26.503	94.080	28.067	1.00	30.18
	2448	CA	VAL	B	445	25.530	93.168	28.650	1.00	28.24
	2449	C	VAL	B	445	24.077	93.464	28.289	1.00	28.44
	2450	O	VAL	B	445	23.625	94.600	28.379	1.00	26.78
	2451	CB	VAL	B	445	25.663	93.183	30.195	1.00	28.10

	2452	CG1	VAL	B	445	24.667	92.230	30.826	1.00	25.56
	2453	CG2	VAL	B	445	27.079	92.629	30.589	1.00	26.30
	2454	N	TYR	B	446	23.349	92.425	27.897	1.00	27.87
	2455	CA	TYR	B	446	21.949	92.581	27.549	1.00	27.91
	2456	C	TYR	B	446	21.140	91.407	28.076	1.00	27.06
	2457	O	TYR	B	446	21.293	90.274	27.620	1.00	27.96
	2458	CB	TYR	B	446	21.764	92.702	26.026	1.00	26.45
	2459	CG	TYR	B	446	20.311	92.851	25.653	1.00	26.59
	2460	CD1	TYR	B	446	19.543	93.886	26.195	1.00	28.48
	2461	CD2	TYR	B	446	19.686	91.941	24.795	1.00	29.02
	2462	CE1	TYR	B	446	18.183	94.011	25.896	1.00	33.24
	2463	CE2	TYR	B	446	18.326	92.057	24.484	1.00	31.33
	2464	CZ	TYR	B	446	17.585	93.094	25.041	1.00	36.01
	2465	OH	TYR	B	446	16.248	93.213	24.762	1.00	36.54
	2466	N	ALA	B	447	20.274	91.686	29.040	1.00	28.07
	2467	CA	ALA	B	447	19.450	90.651	29.661	1.00	27.67
	2468	C	ALA	B	447	18.021	90.785	29.168	1.00	29.19
	2469	O	ALA	B	447	17.564	91.898	28.927	1.00	31.10
	2470	CB	ALA	B	447	19.502	90.798	31.169	1.00	23.97
	2471	N	PHE	B	448	17.307	89.671	29.021	1.00	29.56
	2472	CA	PHE	B	448	15.943	89.751	28.522	1.00	32.50
	2473	C	PHE	B	448	15.117	88.525	28.854	1.00	33.67
	2474	O	PHE	B	448	15.650	87.488	29.228	1.00	35.26
	2475	CB	PHE	B	448	15.970	89.941	27.003	1.00	35.29
	2476	CG	PHE	B	448	16.523	88.751	26.262	1.00	37.04
	2477	CD1	PHE	B	448	15.691	87.688	25.905	1.00	36.66
	2478	CD2	PHE	B	448	17.886	88.666	25.973	1.00	34.95
	2479	CE1	PHE	B	448	16.218	86.551	25.276	1.00	40.91
	2480	CE2	PHE	B	448	18.422	87.534	25.347	1.00	35.99
	2481	CZ	PHE	B	448	17.586	86.477	24.997	1.00	35.15
	2482	N	ALA	B	449	13.804	88.648	28.704	1.00	35.81
	2483	CA	ALA	B	449	12.907	87.534	28.969	1.00	37.63
	2484	C	ALA	B	449	12.347	86.983	27.662	1.00	40.96
	2485	O	ALA	B	449	12.159	87.715	26.697	1.00	40.14
	2486	CB	ALA	B	449	11.769	87.977	29.870	1.00	33.60
	2487	N	THR	B	450	12.091	85.682	27.652	1.00	45.40
	2488	CA	THR	B	450	11.529	84.994	26.505	1.00	50.82
	2489	C	THR	B	450	10.003	85.085	26.602	1.00	53.78
	2490	O	THR	B	450	9.431	84.927	27.683	1.00	54.14
	2491	CB	THR	B	450	11.935	83.510	26.513	1.00	51.45
	2492	OG1	THR	B	450	13.358	83.408	26.650	1.00	54.12
	2493	CG2	THR	B	450	11.507	82.831	25.223	1.00	55.58
	2494	N	PRO	B	451	9.325	85.340	25.474	1.00	56.74
	2495	CA	PRO	B	451	7.863	85.443	25.477	1.00	59.05
	2496	C	PRO	B	451	7.209	84.173	26.020	1.00	61.00
	2497	O	PRO	B	451	7.520	83.065	25.579	1.00	59.71
	2498	CB	PRO	B	451	7.527	85.667	24.002	1.00	60.52
	2499	CG	PRO	B	451	8.749	86.338	23.460	1.00	61.14
	2500	CD	PRO	B	451	9.861	85.551	24.119	1.00	59.39
	2501	N	GLU	B	452	6.315	84.328	26.988	1.00	64.30
	2502	CA	GLU	B	452	5.625	83.172	27.542	1.00	69.17
	2503	C	GLU	B	452	4.137	83.348	27.258	1.00	72.61
	2504	O	GLU	B	452	3.394	83.933	28.043	1.00	73.59
	2505	CB	GLU	B	452	5.888	83.040	29.046	1.00	65.66
	2506	CG	GLU	B	452	6.034	81.585	29.523	1.00	61.46
	2507	CD	GLU	B	452	7.283	80.883	28.967	1.00	60.52
	2508	OE1	GLU	B	452	8.336	81.547	28.849	1.00	63.47
	2509	OE2	GLU	B	452	7.227	79.666	28.667	1.00	53.34
	2510	N	TRP	B	453	3.731	82.837	26.103	1.00	76.75
	2511	CA	TRP	B	453	2.358	82.907	25.619	1.00	81.00
	2512	C	TRP	B	453	1.573	81.714	26.187	1.00	82.30
	2513	O	TRP	B	453	1.890	80.562	25.885	1.00	82.08

	2514	CB	TRP	B	453	2.409	82.863	24.090	1.00	85.65
	2515	CG	TRP	B	453	1.233	83.418	23.366	1.00	89.76
	2516	CD1	TRP	B	453	0.679	84.661	23.512	1.00	92.34
	2517	CD2	TRP	B	453	0.517	82.781	22.305	1.00	94.15
	2518	NE1	TRP	B	453	-0.334	84.836	22.598	1.00	94.99
	2519	CE2	TRP	B	453	-0.455	83.696	21.845	1.00	95.56
	2520	CE3	TRP	B	453	0.605	81.521	21.693	1.00	95.36
	2521	CZ2	TRP	B	453	-1.335	83.392	20.800	1.00	97.14
	2522	CZ3	TRP	B	453	-0.269	81.220	20.655	1.00	95.61
	2523	CH2	TRP	B	453	-1.226	82.153	20.220	1.00	97.12
	2524	N	PRO	B	454	0.542	81.981	27.020	1.00	84.10
	2525	CA	PRO	B	454	-0.331	80.994	27.678	1.00	87.24
	2526	C	PRO	B	454	-0.716	79.708	26.938	1.00	90.52
	2527	O	PRO	B	454	-0.378	79.512	25.767	1.00	89.75
	2528	CB	PRO	B	454	-1.550	81.825	28.112	1.00	84.91
	2529	CG	PRO	B	454	-1.417	83.125	27.360	1.00	83.62
	2530	CD	PRO	B	454	0.063	83.341	27.307	1.00	84.60
	2531	N	GLY	B	455	-1.455	78.849	27.636	1.00	91.72
	2532	CA	GLY	B	455	-1.813	77.552	27.088	1.00	94.13
	2533	C	GLY	B	455	-0.532	76.870	27.499	1.00	96.28
	2534	O	GLY	B	455	0.475	76.987	26.799	1.00	97.74
	2535	N	SER	B	456	-0.542	76.158	28.622	1.00	99.11
	2536	CA	SER	B	456	0.731	75.626	29.077	1.00	96.15
	2537	C	SER	B	456	1.135	74.193	29.424	1.00	91.50
	2538	O	SER	B	456	0.316	73.308	29.767	1.00	88.52
	2539	CB	SER	B	456	1.222	76.508	30.221	1.00	95.05
	2540	OG	SER	B	456	0.225	76.690	31.216	1.00	110.76
	2541	N	ARG	B	457	2.464	74.059	29.348	1.00	87.73
	2542	CA	ARG	B	457	3.349	72.936	29.580	1.00	87.81
	2543	C	ARG	B	457	4.497	73.922	29.453	1.00	86.30
	2544	O	ARG	B	457	4.602	74.574	28.403	1.00	90.57
	2545	CB	ARG	B	457	3.339	71.966	28.425	1.00	94.67
	2546	N	ASP	B	458	5.341	74.088	30.473	1.00	87.32
	2547	CA	ASP	B	458	6.314	75.159	30.320	1.00	80.43
	2548	C	ASP	B	458	7.637	75.178	31.020	1.00	72.83
	2549	O	ASP	B	458	8.163	74.190	31.501	1.00	73.96
	2550	CB	ASP	B	458	5.615	76.450	30.715	1.00	83.19
	2551	CG	ASP	B	458	5.300	76.498	32.210	1.00	85.09
	2552	OD1	ASP	B	458	4.694	75.535	32.722	1.00	91.25
	2553	OD2	ASP	B	458	5.661	77.492	32.883	1.00	90.84
	2554	N	LYS	B	459	8.149	76.404	31.024	1.00	66.05
	2555	CA	LYS	B	459	9.389	76.818	31.663	1.00	61.75
	2556	C	LYS	B	459	9.617	78.232	31.214	1.00	56.14
	2557	O	LYS	B	459	9.952	78.456	30.054	1.00	56.54
	2558	CB	LYS	B	459	10.569	75.959	31.211	1.00	68.18
	2559	CG	LYS	B	459	10.796	74.799	32.131	1.00	71.85
	2560	CD	LYS	B	459	10.737	75.194	33.601	1.00	73.79
	2561	CE	LYS	B	459	10.761	73.945	34.474	1.00	76.14
	2562	NZ	LYS	B	459	10.925	74.259	35.931	1.00	79.35
	2563	N	ARG	B	460	9.406	79.194	32.099	1.00	52.32
	2564	CA	ARG	B	460	9.649	80.565	31.723	1.00	47.59
	2565	C	ARG	B	460	11.164	80.740	31.810	1.00	43.34
	2566	O	ARG	B	460	11.839	80.123	32.638	1.00	40.40
	2567	CB	ARG	B	460	8.874	81.496	32.644	1.00	49.27
	2568	CG	ARG	B	460	7.384	81.325	32.429	1.00	56.23
	2569	CD	ARG	B	460	6.594	81.941	33.568	1.00	63.20
	2570	NE	ARG	B	460	5.174	81.603	33.504	1.00	68.02
	2571	CZ	ARG	B	460	4.645	80.455	33.920	1.00	70.46
	2572	NH1	ARG	B	460	5.415	79.506	34.444	1.00	72.23
	2573	NH2	ARG	B	460	3.336	80.264	33.815	1.00	73.53
	2574	N	THR	B	461	11.690	81.538	30.902	1.00	39.19
	2575	CA	THR	B	461	13.126	81.721	30.822	1.00	36.81

	2576	C	THR	B	461	13.596	83.153	30.699	1.00	34.03
	2577	O	THR	B	461	12.993	83.969	29.990	1.00	33.96
	2578	CB	THR	B	461	13.710	80.997	29.588	1.00	39.13
	2579	OG1	THR	B	461	13.243	79.643	29.543	1.00	46.04
	2580	CG2	THR	B	461	15.220	80.970	29.679	1.00	45.48
	2581	N	LEU	B	462	14.696	83.443	31.386	1.00	29.84
	2582	CA	LEU	B	462	15.333	84.747	31.312	1.00	28.03
	2583	C	LEU	B	462	16.674	84.395	30.690	1.00	27.33
	2584	O	LEU	B	462	17.186	83.293	30.893	1.00	24.47
	2585	CB	LEU	B	462	15.526	85.377	32.697	1.00	25.97
	2586	CG	LEU	B	462	14.238	85.712	33.465	1.00	33.39
	2587	CD1	LEU	B	462	14.593	86.428	34.781	1.00	32.36
	2588	CD2	LEU	B	462	13.337	86.586	32.617	1.00	30.72
	2589	N	ALA	B	463	17.241	85.314	29.922	1.00	25.83
	2590	CA	ALA	B	463	18.489	85.023	29.264	1.00	25.65
	2591	C	ALA	B	463	19.321	86.270	29.143	1.00	26.32
	2592	O	ALA	B	463	18.810	87.386	29.254	1.00	27.53
	2593	CB	ALA	B	463	18.219	84.421	27.888	1.00	28.15
	2594	N	CYS	B	464	20.608	86.082	28.905	1.00	21.23
	2595	CA	CYS	B	464	21.507	87.212	28.824	1.00	24.77
	2596	C	CYS	B	464	22.584	87.001	27.786	1.00	22.14
	2597	O	CYS	B	464	23.169	85.917	27.698	1.00	24.66
	2598	CB	CYS	B	464	22.171	87.407	30.186	1.00	22.04
	2599	SG	CYS	B	464	23.302	88.810	30.380	1.00	34.06
	2600	N	LEU	B	465	22.859	88.052	27.025	1.00	22.44
	2601	CA	LEU	B	465	23.903	88.002	26.011	1.00	23.11
	2602	C	LEU	B	465	24.985	88.956	26.459	1.00	22.43
	2603	O	LEU	B	465	24.702	90.117	26.748	1.00	23.73
	2604	CB	LEU	B	465	23.370	88.445	24.639	1.00	22.99
	2605	CG	LEU	B	465	24.423	88.790	23.562	1.00	19.04
	2606	CD1	LEU	B	465	25.269	87.565	23.234	1.00	21.72
	2607	CD2	LEU	B	465	23.716	89.253	22.282	1.00	28.23
	2608	N	ILE	B	466	26.220	88.475	26.519	1.00	22.56
	2609	CA	ILE	B	466	27.332	89.323	26.931	1.00	22.11
	2610	C	ILE	B	466	28.344	89.298	25.803	1.00	24.25
	2611	O	ILE	B	466	28.785	88.225	25.394	1.00	24.93
	2612	CB	ILE	B	466	27.946	88.819	28.239	1.00	22.15
	2613	CG1	ILE	B	466	26.850	88.751	29.314	1.00	23.07
	2614	CG2	ILE	B	466	29.075	89.778	28.684	1.00	25.24
	2615	CD1	ILE	B	466	27.282	88.091	30.604	1.00	33.12
	2616	N	GLN	B	467	28.737	90.468	25.307	1.00	24.63
	2617	CA	GLN	B	467	29.630	90.480	24.149	1.00	28.64
	2618	C	GLN	B	467	30.637	91.618	24.028	1.00	31.08
	2619	O	GLN	B	467	30.685	92.529	24.865	1.00	31.00
	2620	CB	GLN	B	467	28.770	90.428	22.872	1.00	25.58
	2621	CG	GLN	B	467	27.873	91.657	22.696	1.00	25.53
	2622	CD	GLN	B	467	26.907	91.556	21.501	1.00	30.72
	2623	OE1	GLN	B	467	27.144	90.810	20.551	1.00	29.76
	2624	NE2	GLN	B	467	25.821	92.327	21.550	1.00	32.18
	2625	N	ASN	B	468	31.453	91.517	22.977	1.00	33.71
	2626	CA	ASN	B	468	32.494	92.486	22.641	1.00	36.96
	2627	C	ASN	B	468	33.601	92.607	23.677	1.00	38.20
	2628	O	ASN	B	468	34.208	93.669	23.812	1.00	38.39
	2629	CB	ASN	B	468	31.881	93.869	22.424	1.00	41.06
	2630	CG	ASN	B	468	30.763	93.852	21.414	1.00	46.41
	2631	OD1	ASN	B	468	30.879	93.228	20.359	1.00	50.82
	2632	ND2	ASN	B	468	29.672	94.548	21.724	1.00	53.31
	2633	N	PHE	B	469	33.868	91.535	24.415	1.00	35.74
	2634	CA	PHE	B	469	34.910	91.597	25.423	1.00	33.87
	2635	C	PHE	B	469	36.147	90.796	25.044	1.00	33.63
	2636	O	PHE	B	469	36.087	89.873	24.240	1.00	34.78
	2637	CB	PHE	B	469	34.372	91.105	26.778	1.00	29.12

	2638	CG	PHE	B	469	33.909	89.674	26.766	1.00	26.27
	2639	CD1	PHE	B	469	34.808	88.641	26.967	1.00	22.45
	2640	CD2	PHE	B	469	32.566	89.362	26.561	1.00	22.06
	2641	CE1	PHE	B	469	34.386	87.315	26.974	1.00	23.84
	2642	CE2	PHE	B	469	32.135	88.036	26.564	1.00	28.02
	2643	CZ	PHE	B	469	33.051	87.007	26.773	1.00	23.33
	2644	N	MET	B	470	37.273	91.169	25.634	1.00	35.64
	2645	CA	MET	B	470	38.535	90.480	25.413	1.00	37.62
	2646	C	MET	B	470	39.496	90.916	26.504	1.00	36.36
	2647	O	MET	B	470	39.478	92.071	26.923	1.00	36.33
	2648	CB	MET	B	470	39.105	90.796	24.024	1.00	42.61
	2649	CG	MET	B	470	39.421	92.246	23.750	1.00	50.60
	2650	SD	MET	B	470	39.856	92.459	21.987	1.00	66.08
	2651	CE	MET	B	470	41.544	91.820	21.966	1.00	66.35
	2652	N	PRO	B	471	40.317	89.987	27.021	1.00	34.63
	2653	CA	PRO	B	471	40.431	88.561	26.682	1.00	32.61
	2654	C	PRO	B	471	39.147	87.782	26.957	1.00	31.92
	2655	O	PRO	B	471	38.164	88.356	27.415	1.00	29.59
	2656	CB	PRO	B	471	41.585	88.080	27.562	1.00	33.95
	2657	CG	PRO	B	471	42.373	89.323	27.805	1.00	37.90
	2658	CD	PRO	B	471	41.309	90.354	28.042	1.00	34.78
	2659	N	GLU	B	472	39.187	86.472	26.714	1.00	32.28
	2660	CA	GLU	B	472	38.020	85.599	26.866	1.00	36.49
	2661	C	GLU	B	472	37.557	85.220	28.270	1.00	35.52
	2662	O	GLU	B	472	36.438	84.730	28.417	1.00	34.87
	2663	CB	GLU	B	472	38.223	84.298	26.085	1.00	41.97
	2664	CG	GLU	B	472	39.294	83.387	26.677	1.00	54.78
	2665	CD	GLU	B	472	39.456	82.073	25.916	1.00	62.41
	2666	OE1	GLU	B	472	39.021	81.997	24.744	1.00	67.26
	2667	OE2	GLU	B	472	40.034	81.119	26.487	1.00	64.96
	2668	N	ASP	B	473	38.379	85.439	29.295	1.00	34.38
	2669	CA	ASP	B	473	37.971	85.057	30.648	1.00	31.83
	2670	C	ASP	B	473	36.914	85.998	31.214	1.00	31.24
	2671	O	ASP	B	473	37.072	87.220	31.199	1.00	31.80
	2672	CB	ASP	B	473	39.180	84.979	31.584	1.00	34.73
	2673	CG	ASP	B	473	40.147	83.854	31.196	1.00	40.83
	2674	OD1	ASP	B	473	39.676	82.759	30.804	1.00	44.18
	2675	OD2	ASP	B	473	41.378	84.061	31.290	1.00	40.17
	2676	N	ILE	B	474	35.826	85.416	31.702	1.00	26.96
	2677	CA	ILE	B	474	34.744	86.207	32.246	1.00	25.39
	2678	C	ILE	B	474	33.885	85.375	33.208	1.00	24.74
	2679	O	ILE	B	474	33.776	84.164	33.069	1.00	25.20
	2680	CB	ILE	B	474	33.862	86.758	31.092	1.00	23.81
	2681	CG1	ILE	B	474	32.925	87.852	31.598	1.00	22.23
	2682	CG2	ILE	B	474	33.062	85.626	30.453	1.00	27.10
	2683	CD1	ILE	B	474	32.144	88.536	30.450	1.00	25.30
	2684	N	SER	B	475	33.312	86.030	34.209	1.00	23.27
	2685	CA	SER	B	475	32.430	85.348	35.148	1.00	22.17
	2686	C	SER	B	475	31.066	85.991	34.952	1.00	21.71
	2687	O	SER	B	475	30.951	87.207	34.876	1.00	20.84
	2688	CB	SER	B	475	32.879	85.551	36.593	1.00	20.43
	2689	OG	SER	B	475	34.164	85.011	36.806	1.00	30.00
	2690	N	VAL	B	476	30.042	85.158	34.887	1.00	21.76
	2691	CA	VAL	B	476	28.694	85.620	34.675	1.00	21.72
	2692	C	VAL	B	476	27.875	85.165	35.851	1.00	23.56
	2693	O	VAL	B	476	28.036	84.045	36.320	1.00	25.95
	2694	CB	VAL	B	476	28.087	84.994	33.385	1.00	21.56
	2695	CG1	VAL	B	476	26.625	85.443	33.222	1.00	18.70

	2696	CG2	VAL	B	476	28.915	85.403	32.166	1.00	20.99
	2697	N	GLN	B	477	26.994	86.026	36.336	1.00	25.16
	2698	CA	GLN	B	477	26.172	85.635	37.460	1.00	26.65
	2699	C	GLN	B	477	24.833	86.337	37.438	1.00	26.62
	2700	O	GLN	B	477	24.709	87.440	36.925	1.00	26.40
	2701	CB	GLN	B	477	26.917	85.899	38.775	1.00	31.51
	2702	CG	GLN	B	477	27.348	87.311	39.011	1.00	44.27
	2703	CD	GLN	B	477	28.505	87.412	40.016	1.00	47.76
	2704	OE1	GLN	B	477	28.814	88.496	40.502	1.00	50.57
	2705	NE2	GLN	B	477	29.151	86.283	40.313	1.00	47.32
	2706	N	TRP	B	478	23.820	85.659	37.954	1.00	27.41
	2707	CA	TRP	B	478	22.488	86.225	38.026	1.00	28.36
	2708	C	TRP	B	478	22.192	86.656	39.465	1.00	30.10
	2709	O	TRP	B	478	22.660	86.033	40.428	1.00	25.31
	2710	CB	TRP	B	478	21.461	85.196	37.567	1.00	28.76
	2711	CG	TRP	B	478	21.502	84.951	36.087	1.00	34.11
	2712	CD1	TRP	B	478	22.313	84.078	35.415	1.00	31.25
	2713	CD2	TRP	B	478	20.722	85.620	35.094	1.00	31.01
	2714	NE1	TRP	B	478	22.085	84.164	34.069	1.00	27.71
	2715	CE2	TRP	B	478	21.113	85.104	33.841	1.00	31.95
	2716	CE3	TRP	B	478	19.729	86.607	35.140	1.00	34.16
	2717	CZ2	TRP	B	478	20.542	85.545	32.637	1.00	25.26
	2718	CZ3	TRP	B	478	19.161	87.044	33.947	1.00	31.64
	2719	CH2	TRP	B	478	19.571	86.511	32.713	1.00	28.89
	2720	N	LEU	B	479	21.418	87.723	39.602	1.00	32.48
	2721	CA	LEU	B	479	21.049	88.245	40.913	1.00	37.36
	2722	C	LEU	B	479	19.584	88.657	40.960	1.00	40.42
	2723	O	LEU	B	479	19.040	89.152	39.977	1.00	40.14
	2724	CB	LEU	B	479	21.878	89.478	41.252	1.00	39.83
	2725	CG	LEU	B	479	23.346	89.556	40.842	1.00	44.57
	2726	CD1	LEU	B	479	23.890	90.887	41.290	1.00	52.98
	2727	CD2	LEU	B	479	24.130	88.439	41.466	1.00	50.71
	2728	N	HIS	B	480	18.947	88.448	42.102	1.00	43.05
	2729	CA	HIS	B	480	17.572	88.877	42.276	1.00	49.20
	2730	C	HIS	B	480	17.746	90.136	43.116	1.00	52.73
	2731	O	HIS	B	480	17.705	90.091	44.347	1.00	52.90
	2732	CB	HIS	B	480	16.754	87.844	43.043	1.00	52.25
	2733	CG	HIS	B	480	15.341	88.270	43.286	1.00	57.22
	2734	ND1	HIS	B	480	14.337	88.075	42.364	1.00	61.37
	2735	CD2	HIS	B	480	14.778	88.942	44.319	1.00	59.16
	2736	CE1	HIS	B	480	13.216	88.607	42.815	1.00	59.88
	2737	NE2	HIS	B	480	13.456	89.140	44.000	1.00	66.11
	2738	N	ASN	B	481	17.971	91.253	42.430	1.00	56.65
	2739	CA	ASN	B	481	18.206	92.543	43.070	1.00	59.93
	2740	C	ASN	B	481	19.660	92.591	43.519	1.00	59.65
	2741	O	ASN	B	481	20.571	92.569	42.695	1.00	61.04
	2742	CB	ASN	B	481	17.288	92.751	44.282	1.00	64.65
	2743	CG	ASN	B	481	15.852	93.022	43.890	1.00	72.38
	2744	OD1	ASN	B	481	15.563	93.964	43.147	1.00	74.96
	2745	ND2	ASN	B	481	14.938	92.199	44.393	1.00	75.60
	2746	N	GLU	B	482	19.872	92.625	44.827	1.00	58.97
	2747	CA	GLU	B	482	21.213	92.697	45.396	1.00	58.55
	2748	C	GLU	B	482	21.815	91.346	45.782	1.00	55.30
	2749	O	GLU	B	482	23.013	91.253	46.044	1.00	57.27
	2750	CB	GLU	B	482	21.176	93.607	46.627	1.00	65.42
	2751	CG	GLU	B	482	19.760	93.813	47.172	1.00	73.94
	2752	CD	GLU	B	482	19.735	94.473	48.532	1.00	80.29
	2753	OE1	GLU	B	482	20.168	93.830	49.513	1.00	86.31
	2754	OE2	GLU	B	482	19.284	95.633	48.620	1.00	82.73
	2755	N	VAL	B	483	20.997	90.301	45.814	1.00	50.25
	2756	CA	VAL	B	483	21.487	88.988	46.211	1.00	45.78
	2757	C	VAL	B	483	21.733	88.025	45.052	1.00	43.04

	2758	O	VAL	B	483	20.880	87.834	44.198	1.00	41.34
	2759	CB	VAL	B	483	20.527	88.339	47.233	1.00	43.76
	2760	CG1	VAL	B	483	19.129	88.283	46.668	1.00	46.25
	2761	CG2	VAL	B	483	21.011	86.946	47.594	1.00	41.37
	2762	N	GLN	B	484	22.912	87.412	45.050	1.00	42.30
	2763	CA	GLN	B	484	23.300	86.474	44.005	1.00	43.21
	2764	C	GLN	B	484	22.658	85.091	44.141	1.00	42.48
	2765	O	GLN	B	484	22.538	84.545	45.244	1.00	41.64
	2766	CB	GLN	B	484	24.826	86.331	43.971	1.00	45.96
	2767	CG	GLN	B	484	25.324	85.269	42.999	1.00	54.43
	2768	CD	GLN	B	484	26.840	85.173	42.941	1.00	59.02
	2769	OE1	GLN	B	484	27.391	84.200	42.423	1.00	59.71
	2770	NE2	GLN	B	484	27.522	86.190	43.464	1.00	61.46
	2771	N	LEU	B	485	22.239	84.539	43.006	1.00	38.99
	2772	CA	LEU	B	485	21.618	83.218	42.953	1.00	39.17
	2773	C	LEU	B	485	22.700	82.142	42.853	1.00	40.35
	2774	O	LEU	B	485	23.822	82.417	42.430	1.00	37.39
	2775	CB	LEU	B	485	20.705	83.107	41.725	1.00	37.16
	2776	CG	LEU	B	485	19.579	84.140	41.602	1.00	39.66
	2777	CD1	LEU	B	485	18.836	83.930	40.293	1.00	39.30
	2778	CD2	LEU	B	485	18.644	84.020	42.795	1.00	40.56
	2779	N	PRO	B	486	22.373	80.900	43.242	1.00	42.55
	2780	CA	PRO	B	486	23.366	79.828	43.158	1.00	46.30
	2781	C	PRO	B	486	23.750	79.660	41.688	1.00	49.32
	2782	O	PRO	B	486	22.916	79.852	40.806	1.00	48.81
	2783	CB	PRO	B	486	22.606	78.609	43.675	1.00	45.64
	2784	CG	PRO	B	486	21.532	79.187	44.528	1.00	45.29
	2785	CD	PRO	B	486	21.095	80.394	43.769	1.00	40.65
	2786	N	ASP	B	487	24.997	79.290	41.429	1.00	53.39
	2787	CA	ASP	B	487	25.465	79.093	40.062	1.00	57.75
	2788	C	ASP	B	487	24.660	77.997	39.350	1.00	57.25
	2789	O	ASP	B	487	24.205	78.176	38.213	1.00	57.75
	2790	CB	ASP	B	487	26.944	78.708	40.077	1.00	67.82
	2791	CG	ASP	B	487	27.577	78.779	38.703	1.00	76.17
	2792	OD1	ASP	B	487	26.945	78.309	37.734	1.00	84.77
	2793	OD2	ASP	B	487	28.711	79.297	38.592	1.00	86.94
	2794	N	ALA	B	488	24.478	76.873	40.035	1.00	54.64
	2795	CA	ALA	B	488	23.752	75.729	39.493	1.00	53.45
	2796	C	ALA	B	488	22.421	76.069	38.837	1.00	52.74
	2797	O	ALA	B	488	21.843	75.241	38.134	1.00	53.06
	2798	CB	ALA	B	488	23.530	74.708	40.585	1.00	53.75
	2799	N	ARG	B	489	21.938	77.287	39.056	1.00	50.96
	2800	CA	ARG	B	489	20.660	77.704	38.491	1.00	47.84
	2801	C	ARG	B	489	20.705	78.164	37.036	1.00	45.10
	2802	O	ARG	B	489	19.681	78.158	36.363	1.00	43.37
	2803	CB	ARG	B	489	20.046	78.808	39.354	1.00	48.99
	2804	CG	ARG	B	489	19.232	78.294	40.524	1.00	50.01
	2805	CD	ARG	B	489	17.761	78.427	40.227	1.00	50.36
	2806	NE	ARG	B	489	17.187	79.581	40.905	1.00	56.65
	2807	CZ	ARG	B	489	16.048	80.166	40.557	1.00	58.23
	2808	NH1	ARG	B	489	15.352	79.714	39.522	1.00	61.07
	2809	NH2	ARG	B	489	15.594	81.193	41.260	1.00	59.63
	2810	N	HIS	B	490	21.872	78.573	36.551	1.00	42.41
	2811	CA	HIS	B	490	21.965	79.024	35.166	1.00	41.63
	2812	C	HIS	B	490	22.952	78.210	34.334	1.00	39.71
	2813	O	HIS	B	490	23.768	77.471	34.865	1.00	41.30
	2814	CB	HIS	B	490	22.348	80.508	35.100	1.00	42.40
	2815	CG	HIS	B	490	23.720	80.807	35.614	1.00	43.27
	2816	ND1	HIS	B	490	23.966	81.177	36.919	1.00	42.27
	2817	CD2	HIS	B	490	24.926	80.779	34.999	1.00	44.41
	2818	CE1	HIS	B	490	25.262	81.364	37.086	1.00	39.88
	2819	NE2	HIS	B	490	25.868	81.130	35.934	1.00	45.37

	2820	N	SER	B	491	22.858	78.355	33.020	1.00	37.20
	2821	CA	SER	B	491	23.734	77.654	32.095	1.00	36.36
	2822	C	SER	B	491	24.401	78.685	31.173	1.00	33.06
	2823	O	SER	B	491	23.721	79.428	30.461	1.00	33.77
	2824	CB	SER	B	491	22.910	76.651	31.288	1.00	35.42
	2825	OG	SER	B	491	23.694	76.053	30.282	1.00	43.65
	2826	N	THR	B	492	25.728	78.722	31.188	1.00	29.90
	2827	CA	THR	B	492	26.495	79.673	30.383	1.00	29.91
	2828	C	THR	B	492	27.322	78.977	29.287	1.00	29.20
	2829	O	THR	B	492	27.996	77.991	29.552	1.00	30.85
	2830	CB	THR	B	492	27.447	80.506	31.298	1.00	29.85
	2831	OG1	THR	B	492	26.670	81.197	32.281	1.00	35.86
	2832	CG2	THR	B	492	28.234	81.541	30.498	1.00	28.05
	2833	N	THR	B	493	27.281	79.505	28.065	1.00	29.49
	2834	CA	THR	B	493	28.032	78.913	26.957	1.00	30.19
	2835	C	THR	B	493	29.501	79.295	27.056	1.00	32.39
	2836	O	THR	B	493	29.863	80.210	27.786	1.00	30.70
	2837	CB	THR	B	493	27.502	79.378	25.568	1.00	27.82
	2838	OG1	THR	B	493	27.592	80.806	25.460	1.00	30.48
	2839	CG2	THR	B	493	26.067	78.953	25.372	1.00	22.03
	2840	N	GLN	B	494	30.347	78.586	26.322	1.00	35.09
	2841	CA	GLN	B	494	31.779	78.879	26.330	1.00	38.19
	2842	C	GLN	B	494	32.032	80.091	25.449	1.00	36.48
	2843	O	GLN	B	494	31.360	80.270	24.432	1.00	35.75
	2844	CB	GLN	B	494	32.581	77.696	25.775	1.00	43.09
	2845	CG	GLN	B	494	32.502	76.433	26.610	1.00	58.35
	2846	CD	GLN	B	494	32.929	76.666	28.042	1.00	65.11
	2847	OE1	GLN	B	494	34.003	77.209	28.303	1.00	71.67
	2848	NE2	GLN	B	494	32.088	76.255	28.982	1.00	71.87
	2849	N	PRO	B	495	33.002	80.939	25.828	1.00	36.89
	2850	CA	PRO	B	495	33.322	82.130	25.037	1.00	38.37
	2851	C	PRO	B	495	33.609	81.737	23.587	1.00	40.80
	2852	O	PRO	B	495	34.314	80.763	23.327	1.00	40.76
	2853	CB	PRO	B	495	34.557	82.680	25.729	1.00	37.83
	2854	CG	PRO	B	495	34.315	82.300	27.174	1.00	40.41
	2855	CD	PRO	B	495	33.809	80.884	27.061	1.00	35.81
	2856	N	ARG	B	496	33.040	82.480	22.650	1.00	42.05
	2857	CA	ARG	B	496	33.255	82.208	21.240	1.00	47.69
	2858	C	ARG	B	496	33.772	83.454	20.542	1.00	51.66
	2859	O	ARG	B	496	33.283	84.558	20.784	1.00	51.95
	2860	CB	ARG	B	496	31.954	81.751	20.584	1.00	45.81
	2861	CG	ARG	B	496	31.599	80.317	20.892	1.00	51.53
	2862	CD	ARG	B	496	30.217	79.947	20.391	1.00	53.72
	2863	NE	ARG	B	496	30.175	78.554	19.963	1.00	57.50
	2864	CZ	ARG	B	496	30.608	78.122	18.783	1.00	58.59
	2865	NH1	ARG	B	496	31.111	78.974	17.901	1.00	57.22
	2866	NH2	ARG	B	496	30.542	76.832	18.488	1.00	65.31
	2867	N	LYS	B	497	34.773	83.281	19.687	1.00	56.98
	2868	CA	LYS	B	497	35.335	84.408	18.953	1.00	61.91
	2869	C	LYS	B	497	34.301	84.867	17.955	1.00	63.97
	2870	O	LYS	B	497	33.300	84.195	17.729	1.00	64.61
	2871	CB	LYS	B	497	36.587	84.003	18.172	1.00	66.35
	2872	CG	LYS	B	497	37.848	83.781	18.987	1.00	74.14
	2873	CD	LYS	B	497	38.993	83.359	18.066	1.00	80.69
	2874	CE	LYS	B	497	40.304	83.192	18.814	1.00	84.48
	2875	NZ	LYS	B	497	41.385	82.739	17.889	1.00	88.26
	2876	N	THR	B	498	34.555	86.017	17.352	1.00	67.67
	2877	CA	THR	B	498	33.669	86.572	16.342	1.00	71.26
	2878	C	THR	B	498	34.550	87.284	15.340	1.00	73.04
	2879	O	THR	B	498	35.743	86.990	15.236	1.00	72.83
	2880	CB	THR	B	498	32.679	87.585	16.945	1.00	71.80
	2881	OG1	THR	B	498	33.392	88.555	17.721	1.00	71.58

	2882	CG2	THR	B	498	31.670	86.878	17.819	1.00	73.61
	2883	N	LYS	B	499	33.962	88.220	14.605	1.00	75.57
	2884	CA	LYS	B	499	34.705	88.993	13.620	1.00	77.62
	2885	C	LYS	B	499	35.427	90.142	14.321	1.00	77.92
	2886	O	LYS	B	499	34.791	91.096	14.768	1.00	79.19
	2887	CB	LYS	B	499	33.752	89.558	12.567	1.00	80.22
	2888	CG	LYS	B	499	33.172	88.531	11.604	1.00	81.04
	2889	CD	LYS	B	499	34.203	88.093	10.571	1.00	83.26
	2890	CE	LYS	B	499	33.569	87.232	9.487	1.00	84.81
	2891	NZ	LYS	B	499	34.545	86.864	8.425	1.00	86.04
	2892	N	GLY	B	500	36.748	90.034	14.433	1.00	76.91
	2893	CA	GLY	B	500	37.544	91.077	15.061	1.00	75.83
	2894	C	GLY	B	500	37.141	91.560	16.445	1.00	75.14
	2895	O	GLY	B	500	37.971	91.576	17.355	1.00	75.52
	2896	N	SER	B	501	35.882	91.958	16.605	1.00	73.08
	2897	CA	SER	B	501	35.370	92.468	17.875	1.00	71.65
	2898	C	SER	B	501	36.008	91.836	19.106	1.00	68.64
	2899	O	SER	B	501	36.690	92.515	19.877	1.00	71.13
	2900	CB	SER	B	501	33.854	92.279	17.953	1.00	74.43
	2901	OG	SER	B	501	33.524	90.933	18.241	1.00	80.92
	2902	N	GLY	B	502	35.786	90.540	19.290	1.00	63.14
	2903	CA	GLY	B	502	36.344	89.859	20.443	1.00	54.62
	2904	C	GLY	B	502	35.552	88.618	20.803	1.00	48.04
	2905	O	GLY	B	502	35.469	87.683	20.006	1.00	48.08
	2906	N	PHE	B	503	34.958	88.599	21.994	1.00	40.50
	2907	CA	PHE	B	503	34.189	87.427	22.408	1.00	33.81
	2908	C	PHE	B	503	32.773	87.692	22.888	1.00	28.39
	2909	O	PHE	B	503	32.408	88.811	23.244	1.00	26.35
	2910	CB	PHE	B	503	34.919	86.662	23.517	1.00	35.09
	2911	CG	PHE	B	503	36.263	86.148	23.119	1.00	34.16
	2912	CD1	PHE	B	503	37.381	86.970	23.174	1.00	35.05
	2913	CD2	PHE	B	503	36.411	84.845	22.670	1.00	35.90
	2914	CE1	PHE	B	503	38.633	86.501	22.783	1.00	36.00
	2915	CE2	PHE	B	503	37.656	84.362	22.274	1.00	40.04
	2916	CZ	PHE	B	503	38.771	85.192	22.329	1.00	38.82
	2917	N	PHE	B	504	31.975	86.633	22.884	1.00	26.16
	2918	CA	PHE	B	504	30.612	86.709	23.369	1.00	25.00
	2919	C	PHE	B	504	30.286	85.418	24.096	1.00	26.57
	2920	O	PHE	B	504	30.892	84.379	23.833	1.00	26.73
	2921	CB	PHE	B	504	29.616	86.960	22.242	1.00	22.46
	2922	CG	PHE	B	504	29.330	85.766	21.382	1.00	27.70
	2923	CD1	PHE	B	504	28.260	84.926	21.667	1.00	28.94
	2924	CD2	PHE	B	504	30.086	85.517	20.243	1.00	31.34
	2925	CE1	PHE	B	504	27.938	83.857	20.827	1.00	30.08
	2926	CE2	PHE	B	504	29.772	84.449	19.396	1.00	32.65
	2927	CZ	PHE	B	504	28.691	83.621	19.697	1.00	32.80
	2928	N	VAL	B	505	29.330	85.509	25.015	1.00	23.68
	2929	CA	VAL	B	505	28.895	84.389	25.814	1.00	24.67
	2930	C	VAL	B	505	27.385	84.559	26.028	1.00	23.86
	2931	O	VAL	B	505	26.875	85.672	26.051	1.00	21.24
	2932	CB	VAL	B	505	29.674	84.392	27.161	1.00	27.95
	2933	CG1	VAL	B	505	29.136	85.466	28.080	1.00	25.61
	2934	CG2	VAL	B	505	29.643	83.042	27.786	1.00	33.51
	2935	N	PHE	B	506	26.664	83.454	26.141	1.00	26.20
	2936	CA	PHE	B	506	25.218	83.514	26.346	1.00	26.10
	2937	C	PHE	B	506	24.855	82.754	27.621	1.00	24.83
	2938	O	PHE	B	506	25.369	81.672	27.859	1.00	25.52
	2939	CB	PHE	B	506	24.496	82.875	25.161	1.00	28.18
	2940	CG	PHE	B	506	23.007	82.842	25.303	1.00	35.33
	2941	CD1	PHE	B	506	22.245	83.980	25.080	1.00	42.56
	2942	CD2	PHE	B	506	22.359	81.663	25.657	1.00	40.04
	2943	CE1	PHE	B	506	20.854	83.940	25.208	1.00	44.70

	2944	CE2	PHE	B	506	20.977	81.613	25.789	1.00	40.54
	2945	CZ	PHE	B	506	20.223	82.749	25.564	1.00	42.12
	2946	N	SER	B	507	23.961	83.310	28.427	1.00	24.69
	2947	CA	SER	B	507	23.550	82.659	29.674	1.00	24.73
	2948	C	SER	B	507	22.022	82.535	29.745	1.00	26.40
	2949	O	SER	B	507	21.308	83.487	29.491	1.00	25.99
	2950	CB	SER	B	507	24.079	83.449	30.879	1.00	22.19
	2951	OG	SER	B	507	23.653	82.860	32.091	1.00	30.30
	2952	N	ARG	B	508	21.538	81.345	30.091	1.00	26.98
	2953	CA	ARG	B	508	20.104	81.055	30.187	1.00	25.95
	2954	C	ARG	B	508	19.689	80.749	31.637	1.00	24.97
	2955	O	ARG	B	508	20.350	79.979	32.315	1.00	24.35
	2956	CB	ARG	B	508	19.799	79.845	29.310	1.00	21.97
	2957	CG	ARG	B	508	18.365	79.351	29.344	1.00	25.32
	2958	CD	ARG	B	508	18.228	78.126	28.444	1.00	25.67
	2959	NE	ARG	B	508	16.842	77.702	28.312	1.00	36.00
	2960	CZ	ARG	B	508	16.243	76.843	29.128	1.00	36.06
	2961	NH1	ARG	B	508	16.918	76.307	30.137	1.00	34.19
	2962	NH2	ARG	B	508	14.967	76.538	28.943	1.00	34.70
	2963	N	LEU	B	509	18.583	81.331	32.099	1.00	26.44
	2964	CA	LEU	B	509	18.121	81.108	33.479	1.00	28.45
	2965	C	LEU	B	509	16.627	80.806	33.560	1.00	28.87
	2966	O	LEU	B	509	15.803	81.707	33.401	1.00	30.99
	2967	CB	LEU	B	509	18.423	82.341	34.342	1.00	27.28
	2968	CG	LEU	B	509	17.867	82.330	35.779	1.00	31.90
	2969	CD1	LEU	B	509	18.615	81.316	36.647	1.00	29.48
	2970	CD2	LEU	B	509	18.001	83.714	36.368	1.00	28.89
	2971	N	GLU	B	510	16.277	79.546	33.812	1.00	31.92
	2972	CA	GLU	B	510	14.872	79.152	33.911	1.00	34.67
	2973	C	GLU	B	510	14.310	79.595	35.255	1.00	36.35
	2974	O	GLU	B	510	14.948	79.401	36.288	1.00	34.66
	2975	CB	GLU	B	510	14.725	77.630	33.757	1.00	41.07
	2976	CG	GLU	B	510	15.217	77.090	32.404	1.00	54.35
	2977	CD	GLU	B	510	14.925	75.603	32.189	1.00	58.86
	2978	OE1	GLU	B	510	15.236	74.789	33.087	1.00	61.22
	2979	OE2	GLU	B	510	14.393	75.251	31.111	1.00	61.34
	2980	N	VAL	B	511	13.121	80.194	35.248	1.00	36.50
	2981	CA	VAL	B	511	12.531	80.665	36.494	1.00	38.05
	2982	C	VAL	B	511	11.084	80.230	36.692	1.00	42.41
	2983	O	VAL	B	511	10.395	79.856	35.732	1.00	41.92
	2984	CB	VAL	B	511	12.588	82.197	36.592	1.00	31.84
	2985	CG1	VAL	B	511	14.015	82.673	36.431	1.00	32.42
	2986	CG2	VAL	B	511	11.687	82.813	35.547	1.00	26.87
	2987	N	THR	B	512	10.633	80.290	37.946	1.00	43.58
	2988	CA	THR	B	512	9.269	79.903	38.292	1.00	48.37
	2989	C	THR	B	512	8.294	80.998	37.899	1.00	50.53
	2990	O	THR	B	512	8.706	82.113	37.584	1.00	51.77
	2991	CB	THR	B	512	9.125	79.644	39.797	1.00	48.57
	2992	OG1	THR	B	512	9.460	80.834	40.519	1.00	46.96
	2993	CG2	THR	B	512	10.046	78.515	40.234	1.00	45.82
	2994	N	ARG	B	513	7.002	80.678	37.912	1.00	53.29
	2995	CA	ARG	B	513	5.971	81.648	37.556	1.00	55.54
	2996	C	ARG	B	513	6.043	82.819	38.523	1.00	55.38
	2997	O	ARG	B	513	5.859	83.977	38.138	1.00	55.22
	2998	CB	ARG	B	513	4.582	81.006	37.636	1.00	59.23
	2999	CG	ARG	B	513	3.563	81.601	36.672	1.00	65.98
	3000	CD	ARG	B	513	3.326	83.081	36.916	1.00	74.12
	3001	NE	ARG	B	513	2.773	83.742	35.735	1.00	80.97
	3002	CZ	ARG	B	513	2.403	85.019	35.687	1.00	83.64
	3003	NH1	ARG	B	513	2.516	85.791	36.760	1.00	86.02
	3004	NH2	ARG	B	513	1.927	85.528	34.557	1.00	85.44
	3005	N	ALA	B	514	6.315	82.501	39.783	1.00	55.03

	3006	CA	ALA	B	514	6.414	83.504	40.832	1.00	55.46
	3007	C	ALA	B	514	7.496	84.539	40.529	1.00	56.10
	3008	O	ALA	B	514	7.210	85.734	40.426	1.00	56.61
	3009	CB	ALA	B	514	6.692	82.825	42.173	1.00	54.05
	3010	N	GLU	B	515	8.741	84.091	40.388	1.00	55.46
	3011	CA	GLU	B	515	9.819	85.025	40.105	1.00	55.34
	3012	C	GLU	B	515	9.649	85.651	38.729	1.00	54.83
	3013	O	GLU	B	515	10.190	86.723	38.456	1.00	52.33
	3014	CB	GLU	B	515	11.187	84.335	40.232	1.00	57.76
	3015	CG	GLU	B	515	11.221	82.884	39.788	1.00	62.58
	3016	CD	GLU	B	515	12.518	82.184	40.163	1.00	63.27
	3017	OE1	GLU	B	515	13.035	82.432	41.271	1.00	64.89
	3018	OE2	GLU	B	515	13.014	81.372	39.359	1.00	66.59
	3019	N	TRP	B	516	8.884	84.992	37.866	1.00	55.79
	3020	CA	TRP	B	516	8.644	85.528	36.534	1.00	57.81
	3021	C	TRP	B	516	7.778	86.782	36.636	1.00	58.51
	3022	O	TRP	B	516	7.778	87.612	35.726	1.00	57.71
	3023	CB	TRP	B	516	7.951	84.499	35.634	1.00	61.48
	3024	CG	TRP	B	516	8.056	84.862	34.187	1.00	66.54
	3025	CD1	TRP	B	516	9.172	84.777	33.403	1.00	67.26
	3026	CD2	TRP	B	516	7.039	85.460	33.375	1.00	69.56
	3027	NE1	TRP	B	516	8.915	85.291	32.154	1.00	71.76
	3028	CE2	TRP	B	516	7.613	85.718	32.110	1.00	70.88
	3029	CE3	TRP	B	516	5.700	85.807	33.593	1.00	70.94
	3030	CZ2	TRP	B	516	6.894	86.308	31.066	1.00	73.50
	3031	CZ3	TRP	B	516	4.982	86.396	32.552	1.00	74.37
	3032	CH2	TRP	B	516	5.584	86.639	31.304	1.00	74.71
	3033	N	GLU	B	517	7.047	86.918	37.744	1.00	59.66
	3034	CA	GLU	B	517	6.191	88.085	37.972	1.00	61.72
	3035	C	GLU	B	517	7.035	89.299	38.354	1.00	59.87
	3036	O	GLU	B	517	6.606	90.441	38.196	1.00	58.60
	3037	CB	GLU	B	517	5.182	87.818	39.097	1.00	68.82
	3038	CG	GLU	B	517	4.284	86.612	38.879	1.00	80.60
	3039	CD	GLU	B	517	3.242	86.452	39.976	1.00	87.42
	3040	OE1	GLU	B	517	3.369	87.128	41.021	1.00	94.80
	3041	OE2	GLU	B	517	2.301	85.645	39.800	1.00	95.35
	3042	N	GLN	B	518	8.234	89.045	38.867	1.00	57.92
	3043	CA	GLN	B	518	9.132	90.120	39.264	1.00	55.74
	3044	C	GLN	B	518	10.416	90.057	38.436	1.00	54.32
	3045	O	GLN	B	518	11.498	90.393	38.924	1.00	52.85
	3046	CB	GLN	B	518	9.454	90.000	40.745	1.00	54.10
	3047	N	LYS	B	519	10.287	89.646	37.176	1.00	52.69
	3048	CA	LYS	B	519	11.448	89.518	36.309	1.00	52.35
	3049	C	LYS	B	519	12.206	90.819	36.159	1.00	51.69
	3050	O	LYS	B	519	13.397	90.822	35.854	1.00	49.61
	3051	CB	LYS	B	519	11.039	88.983	34.937	1.00	54.31
	3052	CG	LYS	B	519	10.205	89.912	34.088	1.00	55.80
	3053	CD	LYS	B	519	9.723	89.162	32.859	1.00	60.32
	3054	CE	LYS	B	519	8.794	90.002	32.011	1.00	64.05
	3055	NZ	LYS	B	519	8.223	89.191	30.898	1.00	70.92
	3056	N	ASP	B	520	11.511	91.924	36.388	1.00	52.66
	3057	CA	ASP	B	520	12.105	93.251	36.288	1.00	54.22
	3058	C	ASP	B	520	13.209	93.396	37.336	1.00	53.07
	3059	O	ASP	B	520	14.075	94.264	37.229	1.00	52.75
	3060	CB	ASP	B	520	11.032	94.311	36.537	1.00	61.14
	3061	CG	ASP	B	520	9.620	93.779	36.308	1.00	71.19
	3062	OD1	ASP	B	520	9.300	93.407	35.155	1.00	76.53
	3063	OD2	ASP	B	520	8.834	93.729	37.283	1.00	72.86
	3064	N	GLU	B	521	13.177	92.533	38.343	1.00	51.01
	3065	CA	GLU	B	521	14.157	92.582	39.416	1.00	50.49
	3066	C	GLU	B	521	15.394	91.714	39.201	1.00	47.73
	3067	O	GLU	B	521	16.372	91.838	39.935	1.00	48.58

	3068	CB	GLU	B	521	13.493	92.200	40.738	1.00	53.54
	3069	CG	GLU	B	521	12.427	93.177	41.199	1.00	60.11
	3070	CD	GLU	B	521	11.705	92.699	42.442	1.00	65.41
	3071	OE1	GLU	B	521	12.361	92.497	43.486	1.00	67.98
	3072	OE2	GLU	B	521	10.471	92.521	42.374	1.00	73.58
	3073	N	PHE	B	522	15.359	90.828	38.213	1.00	42.66
	3074	CA	PHE	B	522	16.519	89.985	37.963	1.00	38.90
	3075	C	PHE	B	522	17.583	90.753	37.208	1.00	35.93
	3076	O	PHE	B	522	17.276	91.579	36.345	1.00	38.85
	3077	CB	PHE	B	522	16.122	88.716	37.214	1.00	36.56
	3078	CG	PHE	B	522	15.419	87.710	38.081	1.00	39.04
	3079	CD1	PHE	B	522	14.106	87.927	38.495	1.00	42.28
	3080	CD2	PHE	B	522	16.087	86.574	38.539	1.00	36.78
	3081	CE1	PHE	B	522	13.468	87.029	39.362	1.00	44.30
	3082	CE2	PHE	B	522	15.461	85.673	39.405	1.00	40.92
	3083	CZ	PHE	B	522	14.146	85.901	39.817	1.00	39.51
	3084	N	ILE	B	523	18.837	90.492	37.555	1.00	31.27
	3085	CA	ILE	B	523	19.959	91.173	36.944	1.00	29.65
	3086	C	ILE	B	523	21.049	90.211	36.483	1.00	29.13
	3087	O	ILE	B	523	21.360	89.236	37.164	1.00	27.36
	3088	CB	ILE	B	523	20.567	92.180	37.937	1.00	34.21
	3089	CG1	ILE	B	523	19.528	93.251	38.282	1.00	37.38
	3090	CG2	ILE	B	523	21.827	92.796	37.364	1.00	34.94
	3091	CD1	ILE	B	523	19.981	94.227	39.354	1.00	38.56
	3092	N	CYS	B	524	21.610	90.498	35.311	1.00	26.34
	3093	CA	CYS	B	524	22.686	89.699	34.739	1.00	27.10
	3094	C	CYS	B	524	23.946	90.500	34.962	1.00	26.67
	3095	O	CYS	B	524	24.010	91.655	34.569	1.00	27.58
	3096	CB	CYS	B	524	22.473	89.497	33.226	1.00	24.27
	3097	SG	CYS	B	524	23.823	88.626	32.363	1.00	37.60
	3098	N	ARG	B	525	24.951	89.886	35.572	1.00	26.37
	3099	CA	ARG	B	525	26.194	90.576	35.856	1.00	26.35
	3100	C	ARG	B	525	27.419	89.887	35.304	1.00	26.72
	3101	O	ARG	B	525	27.561	88.671	35.400	1.00	29.04
	3102	CB	ARG	B	525	26.376	90.748	37.361	1.00	29.81
	3103	CG	ARG	B	525	27.713	91.393	37.728	1.00	35.40
	3104	CD	ARG	B	525	27.652	92.058	39.099	1.00	46.51
	3105	NE	ARG	B	525	27.796	91.113	40.193	1.00	50.77
	3106	CZ	ARG	B	525	27.461	91.379	41.451	1.00	55.09
	3107	NH1	ARG	B	525	26.951	92.565	41.763	1.00	54.58
	3108	NH2	ARG	B	525	27.650	90.464	42.397	1.00	56.77
	3109	N	ALA	B	526	28.311	90.680	34.731	1.00	25.38
	3110	CA	ALA	B	526	29.528	90.142	34.180	1.00	25.38
	3111	C	ALA	B	526	30.721	90.728	34.925	1.00	25.99
	3112	O	ALA	B	526	30.751	91.933	35.210	1.00	25.50
	3113	CB	ALA	B	526	29.629	90.484	32.696	1.00	25.98
	3114	N	VAL	B	527	31.684	89.872	35.259	1.00	25.84
	3115	CA	VAL	B	527	32.895	90.333	35.902	1.00	25.15
	3116	C	VAL	B	527	33.972	90.078	34.880	1.00	26.30
	3117	O	VAL	B	527	34.119	88.958	34.394	1.00	26.20
	3118	CB	VAL	B	527	33.235	89.557	37.177	1.00	24.43
	3119	CG1	VAL	B	527	34.588	89.990	37.661	1.00	26.95
	3120	CG2	VAL	B	527	32.191	89.819	38.251	1.00	28.13
	3121	N	HIS	B	528	34.738	91.115	34.569	1.00	26.24
	3122	CA	HIS	B	528	35.772	91.018	33.564	1.00	29.14
	3123	C	HIS	B	528	36.822	92.102	33.805	1.00	31.86
	3124	O	HIS	B	528	36.509	93.216	34.239	1.00	31.05
	3125	CB	HIS	B	528	35.121	91.172	32.179	1.00	29.03
	3126	CG	HIS	B	528	36.077	91.082	31.035	1.00	29.34
	3127	ND1	HIS	B	528	36.934	92.109	30.696	1.00	33.33
	3128	CD2	HIS	B	528	36.317	90.090	30.144	1.00	28.93
	3129	CE1	HIS	B	528	37.655	91.755	29.651	1.00	26.07

	3130	NE2	HIS	B	528	37.302	90.530	29.295	1.00	32.19
	3131	N	GLU	B	529	38.064	91.757	33.501	1.00	34.08
55	3132	CA	GLU	B	529	39.207	92.636	33.676	1.00	39.76
	3133	C	GLU	B	529	39.110	94.037	33.066	1.00	41.50
	3134	O	GLU	B	529	39.410	95.020	33.740	1.00	41.48
	3135	CB	GLU	B	529	40.462	91.959	33.122	1.00	43.03
	3136	CG	GLU	B	529	41.665	92.898	33.086	1.00	56.19
5	3137	CD	GLU	B	529	42.827	92.361	32.274	1.00	62.66
	3138	OE1	GLU	B	529	43.812	93.111	32.093	1.00	63.52
	3139	OE2	GLU	B	529	42.758	91.198	31.819	1.00	65.43
	3140	N	ALA	B	530	38.703	94.121	31.800	1.00	42.51
	3141	CA	ALA	B	530	38.622	95.399	31.094	1.00	46.03
10	3142	C	ALA	B	530	37.495	96.331	31.504	1.00	49.29
	3143	O	ALA	B	530	37.447	97.476	31.056	1.00	50.87
	3144	CB	ALA	B	530	38.557	95.157	29.587	1.00	39.71
	3145	N	ALA	B	531	36.595	95.849	32.352	1.00	52.89
	3146	CA	ALA	B	531	35.467	96.651	32.798	1.00	56.14
15	3147	C	ALA	B	531	35.801	97.570	33.976	1.00	59.66
	3148	O	ALA	B	531	35.357	97.342	35.096	1.00	61.00
	3149	CB	ALA	B	531	34.305	95.736	33.162	1.00	52.83
	3150	N	SER	B	532	36.588	98.608	33.730	1.00	63.07
	3151	CA	SER	B	532	36.927	99.544	34.795	1.00	66.03
20	3152	C	SER	B	532	35.822	100.594	34.850	1.00	66.08
	3153	O	SER	B	532	35.317	101.031	33.814	1.00	65.35
	3154	CB	SER	B	532	38.270	100.216	34.507	1.00	68.98
	3155	OG	SER	B	532	38.184	101.074	33.384	1.00	74.64
	3156	N	PRO	B	533	35.427	101.019	36.057	1.00	66.51
25	3157	CA	PRO	B	533	35.887	100.669	37.404	1.00	65.99
	3158	C	PRO	B	533	35.374	99.349	37.983	1.00	63.48
	3159	O	PRO	B	533	34.327	98.840	37.582	1.00	64.33
	3160	CB	PRO	B	533	35.397	101.843	38.227	1.00	69.06
	3161	CG	PRO	B	533	34.044	102.061	37.629	1.00	71.08
30	3162	CD	PRO	B	533	34.358	102.030	36.137	1.00	70.23
	3163	N	SER	B	534	36.134	98.817	38.935	1.00	59.21
	3164	CA	SER	B	534	35.796	97.591	39.648	1.00	55.01
	3165	C	SER	B	534	35.452	96.326	38.852	1.00	50.27
	3166	O	SER	B	534	34.725	95.470	39.347	1.00	48.58
35	3167	CB	SER	B	534	34.666	97.894	40.625	1.00	58.20
	3168	OG	SER	B	534	33.587	98.526	39.962	1.00	63.36
	3169	N	GLN	B	535	35.984	96.213	37.639	1.00	44.89
	3170	CA	GLN	B	535	35.771	95.057	36.770	1.00	42.88
	3171	C	GLN	B	535	34.395	94.406	36.823	1.00	41.55
40	3172	O	GLN	B	535	34.279	93.181	36.806	1.00	40.80
	3173	CB	GLN	B	535	36.831	93.967	37.020	1.00	37.08
	3174	CG	GLN	B	535	37.869	94.298	38.044	1.00	47.40
	3175	CD	GLN	B	535	38.684	95.499	37.669	1.00	44.36
	3176	OE1	GLN	B	535	38.862	96.407	38.475	1.00	47.59
45	3177	NE2	GLN	B	535	39.185	95.521	36.436	1.00	54.70
	3178	N	THR	B	536	33.348	95.213	36.874	1.00	39.97
	3179	CA	THR	B	536	32.012	94.650	36.893	1.00	40.62
	3180	C	THR	B	536	31.025	95.487	36.077	1.00	37.57
	3181	O	THR	B	536	31.042	96.707	36.125	1.00	40.85
50	3182	CB	THR	B	536	31.508	94.463	38.353	1.00	42.38
	3183	OG1	THR	B	536	30.112	94.142	38.337	1.00	44.59
	3184	CG2	THR	B	536	31.730	95.719	39.168	1.00	49.65
	3185	N	VAL	B	537	30.190	94.812	35.299	1.00	35.29
	3186	CA	VAL	B	537	29.182	95.453	34.468	1.00	31.25
55	3187	C	VAL	B	537	27.922	94.604	34.563	1.00	29.01

3188	O	VAL	B	537	27.985	93.382	34.401	1.00	30.11
3189	CB	VAL	B	537	29.604	95.494	32.983	1.00	34.80
3190	CG1	VAL	B	537	28.516	96.148	32.161	1.00	35.52
3191	CG2	VAL	B	537	30.888	96.259	32.822	1.00	37.19
3192	N	GLN	B	538	26.780	95.235	34.808	1.00	26.73
3193	CA	GLN	B	538	25.533	94.493	34.933	1.00	26.74
3194	C	GLN	B	538	24.329	95.224	34.368	1.00	27.53
3195	O	GLN	B	538	24.351	96.431	34.198	1.00	29.89
3196	CB	GLN	B	538	25.265	94.176	36.400	1.00	28.48
3197	CG	GLN	B	538	24.976	95.392	37.266	1.00	25.88
3198	CD	GLN	B	538	24.747	95.005	38.722	1.00	28.51
3199	OE1	GLN	B	538	25.498	94.210	39.290	1.00	31.66
3200	NE2	GLN	B	538	23.715	95.565	39.328	1.00	27.39
3201	N	ARG	B	539	23.266	94.487	34.087	1.00	28.05
3202	CA	ARG	B	539	22.070	95.107	33.565	1.00	30.72
3203	C	ARG	B	539	20.858	94.312	33.986	1.00	31.33
3204	O	ARG	B	539	20.897	93.083	34.023	1.00	32.42
3205	CB	ARG	B	539	22.137	95.180	32.039	1.00	36.30
3206	CG	ARG	B	539	21.124	96.112	31.414	1.00	45.60
3207	CD	ARG	B	539	21.771	96.859	30.270	1.00	57.97
3208	NE	ARG	B	539	23.009	97.482	30.729	1.00	69.46
3209	CZ	ARG	B	539	23.855	98.147	29.950	1.00	78.18
3210	NH1	ARG	B	539	23.604	98.284	28.653	1.00	83.01
3211	NH2	ARG	B	539	24.959	98.673	30.470	1.00	81.89
3212	N	ALA	B	540	19.782	95.022	34.301	1.00	31.92
3213	CA	ALA	B	540	18.546	94.393	34.717	1.00	34.50
3214	C	ALA	B	540	17.826	93.909	33.466	1.00	36.68
3215	O	ALA	B	540	18.068	94.410	32.361	1.00	34.62
3216	CB	ALA	B	540	17.693	95.391	35.479	1.00	33.91
3217	N	VAL	B	541	16.974	92.906	33.640	1.00	39.73
3218	CA	VAL	B	541	16.214	92.346	32.528	1.00	44.47
3219	C	VAL	B	541	15.351	93.436	31.882	1.00	46.91
3220	O	VAL	B	541	14.476	94.005	32.527	1.00	44.53
3221	CB	VAL	B	541	15.305	91.185	33.010	1.00	42.49
3222	CG1	VAL	B	541	14.242	90.885	31.970	1.00	47.96
3223	CG2	VAL	B	541	16.140	89.945	33.269	1.00	42.43
3224	N	SER	B	542	15.603	93.731	30.611	1.00	52.25
3225	CA	SER	B	542	14.829	94.760	29.926	1.00	60.05
3226	C	SER	B	542	13.426	94.226	29.679	1.00	64.25
3227	O	SER	B	542	13.247	93.050	29.357	1.00	65.22
3228	CB	SER	B	542	15.490	95.157	28.600	1.00	60.43
3229	OG	SER	B	542	15.524	94.070	27.696	1.00	65.30
3230	N	VAL	B	543	12.432	95.090	29.844	1.00	68.19
3231	CA	VAL	B	543	11.043	94.694	29.656	1.00	72.45
3232	C	VAL	B	543	10.277	95.772	28.898	1.00	74.32
3233	O	VAL	B	543	9.621	96.630	29.497	1.00	75.99
3234	CB	VAL	B	543	10.353	94.452	31.016	1.00	74.41
3235	CG1	VAL	B	543	8.895	94.070	30.801	1.00	76.37
3236	CG2	VAL	B	543	11.086	93.367	31.782	1.00	75.78

Yet another embodiment of the present invention is a 3-D model of a Fc-Cε3/Cε4 region that substantially represents the atomic coordinates specified (i.e., listed) in Table 3.

Table 3. Atomic coordinates of 1FP5_dimer.pdb with water

ATOM #	ATOM TYPE	RES	CHN	#	X	Y	Z	OCC	B
1	N	VAL	A	336	46.157	62.618	17.991	1.00	58.93
2	CA	VAL	A	336	45.400	61.812	16.993	1.00	60.44
3	C	VAL	A	336	44.013	61.427	17.501	1.00	60.07
4	O	VAL	A	336	43.847	60.389	18.142	1.00	61.48
5	CB	VAL	A	336	46.155	60.521	16.647	1.00	60.81
6	CG1	VAL	A	336	45.464	59.806	15.500	1.00	61.71
7	CG2	VAL	A	336	47.590	60.845	16.302	1.00	64.73
8	N	SER	A	337	43.017	62.257	17.209	1.00	57.95
9	CA	SER	A	337	41.655	61.983	17.648	1.00	56.60
10	C	SER	A	337	40.683	61.842	16.476	1.00	55.17
11	O	SER	A	337	40.981	62.262	15.352	1.00	54.55
12	CB	SER	A	337	41.185	63.078	18.603	1.00	57.92
13	OG	SER	A	337	41.489	64.356	18.087	1.00	64.70
14	N	ALA	A	338	39.527	61.238	16.743	1.00	52.40
15	CA	ALA	A	338	38.522	61.010	15.711	1.00	50.69
16	C	ALA	A	338	37.109	61.300	16.192	1.00	50.25
17	O	ALA	A	338	36.772	61.062	17.354	1.00	51.17
18	CB	ALA	A	338	38.611	59.573	15.211	1.00	50.21
19	N	TYR	A	339	36.281	61.808	15.284	1.00	48.22
20	CA	TYR	A	339	34.899	62.139	15.605	1.00	46.82
21	C	TYR	A	339	33.990	61.766	14.431	1.00	44.51
22	O	TYR	A	339	34.372	61.889	13.268	1.00	42.27
23	CB	TYR	A	339	34.765	63.638	15.915	1.00	50.52
24	CG	TYR	A	339	35.869	64.198	16.793	1.00	58.40
25	CD1	TYR	A	339	37.144	64.445	16.274	1.00	61.23
26	CD2	TYR	A	339	35.648	64.456	18.151	1.00	60.99
27	CE1	TYR	A	339	38.174	64.929	17.081	1.00	62.71
28	CE2	TYR	A	339	36.674	64.943	18.969	1.00	63.53
29	CZ	TYR	A	339	37.933	65.176	18.427	1.00	64.33
30	OH	TYR	A	339	38.953	65.644	19.230	1.00	65.07
31	N	LEU	A	340	32.793	61.291	14.746	1.00	41.90
32	CA	LEU	A	340	31.831	60.905	13.728	1.00	41.06
33	C	LEU	A	340	30.571	61.671	14.078	1.00	41.10
34	O	LEU	A	340	30.136	61.647	15.224	1.00	43.45
35	CB	LEU	A	340	31.583	59.392	13.779	1.00	36.93
36	CG	LEU	A	340	30.689	58.770	12.701	1.00	35.91
37	CD1	LEU	A	340	31.229	59.100	11.314	1.00	34.60
38	CD2	LEU	A	340	30.621	57.264	12.906	1.00	35.51
39	N	SER	A	341	29.990	62.368	13.108	1.00	39.82
40	CA	SER	A	341	28.790	63.152	13.385	1.00	39.85
41	C	SER	A	341	27.598	62.645	12.614	1.00	37.88
42	O	SER	A	341	27.737	62.076	11.544	1.00	42.10
43	CB	SER	A	341	29.025	64.627	13.042	1.00	39.34
44	OG	SER	A	341	29.347	64.792	11.672	1.00	44.58
45	N	ARG	A	342	26.415	62.868	13.158	1.00	36.98
46	CA	ARG	A	342	25.187	62.437	12.517	1.00	35.20
47	C	ARG	A	342	24.853	63.417	11.393	1.00	33.18
48	O	ARG	A	342	25.508	64.443	11.252	1.00	33.16
49	CB	ARG	A	342	24.070	62.394	13.566	1.00	38.57
50	CG	ARG	A	342	24.321	61.381	14.689	1.00	39.10
51	CD	ARG	A	342	23.191	61.364	15.712	1.00	43.21

55	52	NE	ARG	A	342	23.231	62.544	16.570	1.00	45.40
	53	CZ	ARG	A	342	24.086	62.714	17.573	1.00	48.22
	54	NH1	ARG	A	342	24.977	61.777	17.860	1.00	52.78
	55	NH2	ARG	A	342	24.059	63.831	18.286	1.00	54.34
	56	N	PRO	A	343	23.843	63.112	10.570	1.00	33.03
5	57	CA	PRO	A	343	23.497	64.040	9.481	1.00	34.14
	58	C	PRO	A	343	22.907	65.339	10.035	1.00	34.06
	59	O	PRO	A	343	22.302	65.341	11.106	1.00	35.44
	60	CB	PRO	A	343	22.448	63.266	8.667	1.00	33.07
	61	CG	PRO	A	343	22.700	61.811	9.025	1.00	35.06
10	62	CD	PRO	A	343	23.029	61.885	10.499	1.00	33.27
	63	N	SER	A	344	23.080	66.445	9.325	1.00	32.17
	64	CA	SER	A	344	22.490	67.691	9.792	1.00	31.75
	65	C	SER	A	344	21.014	67.617	9.414	1.00	32.07
	66	O	SER	A	344	20.660	67.115	8.344	1.00	30.21
15	67	CB	SER	A	344	23.144	68.907	9.118	1.00	32.20
	68	OG	SER	A	344	22.665	69.113	7.799	1.00	32.50
	69	N	PRO	A	345	20.127	68.088	10.300	1.00	32.31
	70	CA	PRO	A	345	18.701	68.039	9.975	1.00	30.84
	71	C	PRO	A	345	18.381	68.710	8.629	1.00	29.64
20	72	O	PRO	A	345	17.506	68.256	7.891	1.00	30.14
	73	CB	PRO	A	345	18.055	68.741	11.174	1.00	30.96
	74	CG	PRO	A	345	18.941	68.301	12.307	1.00	33.18
	75	CD	PRO	A	345	20.339	68.457	11.713	1.00	33.65
	76	N	PHE	A	346	19.103	69.769	8.292	1.00	28.34
25	77	CA	PHE	A	346	18.844	70.447	7.034	1.00	31.46
	78	C	PHE	A	346	19.085	69.522	5.831	1.00	32.46
	79	O	PHE	A	346	18.269	69.465	4.907	1.00	32.59
	80	CB	PHE	A	346	19.711	71.706	6.916	1.00	32.72
	81	CG	PHE	A	346	19.613	72.382	5.579	1.00	36.34
30	82	CD1	PHE	A	346	18.430	72.981	5.172	1.00	40.58
	83	CD2	PHE	A	346	20.702	72.411	4.722	1.00	36.76
	84	CE1	PHE	A	346	18.333	73.609	3.933	1.00	38.98
	85	CE2	PHE	A	346	20.615	73.037	3.482	1.00	40.15
	86	CZ	PHE	A	346	19.425	73.637	3.086	1.00	38.60
35	87	N	ASP	A	347	20.203	68.797	5.850	1.00	32.92
	88	CA	ASP	A	347	20.534	67.877	4.764	1.00	33.58
	89	C	ASP	A	347	19.555	66.704	4.733	1.00	34.26
	90	O	ASP	A	347	19.192	66.212	3.666	1.00	32.29
	91	CB	ASP	A	347	21.967	67.349	4.921	1.00	28.72
40	92	CG	ASP	A	347	23.008	68.364	4.521	1.00	39.62
	93	OD1	ASP	A	347	24.225	68.085	4.671	1.00	42.08
	94	OD2	ASP	A	347	22.609	69.449	4.046	1.00	46.23
	95	N	LEU	A	348	19.120	66.276	5.911	1.00	34.31
	96	CA	LEU	A	348	18.197	65.159	6.036	1.00	37.70
45	97	C	LEU	A	348	16.742	65.441	5.629	1.00	38.98
	98	O	LEU	A	348	16.137	64.651	4.902	1.00	38.11
	99	CB	LEU	A	348	18.220	64.641	7.482	1.00	40.66
	100	CG	LEU	A	348	17.333	63.441	7.840	1.00	41.99
	101	CD1	LEU	A	348	17.738	62.212	7.005	1.00	42.77
50	102	CD2	LEU	A	348	17.476	63.131	9.341	1.00	41.00
	103	N	PHE	A	349	16.183	66.560	6.083	1.00	39.68
	104	CA	PHE	A	349	14.781	66.875	5.794	1.00	42.09
	105	C	PHE	A	349	14.466	67.883	4.695	1.00	45.09
	106	O	PHE	A	349	13.431	67.779	4.038	1.00	48.27
55	107	CB	PHE	A	349	14.074	67.328	7.071	1.00	37.36
	108	CG	PHE	A	349	14.189	66.356	8.200	1.00	36.93
	109	CD1	PHE	A	349	15.021	66.624	9.282	1.00	38.16

	110	CD2	PHE	A	349	13.487	65.156	8.174	1.00	38.04
	111	CE1	PHE	A	349	15.155	65.715	10.319	1.00	38.11
5	112	CE2	PHE	A	349	13.614	64.231	9.213	1.00	37.58
	113	CZ	PHE	A	349	14.449	64.511	10.283	1.00	40.39
	114	N	ILE	A	350	15.323	68.874	4.500	1.00	46.66
	115	CA	ILE	A	350	15.052	69.854	3.461	1.00	48.94
	116	C	ILE	A	350	15.695	69.400	2.150	1.00	51.15
10	117	O	ILE	A	350	15.007	69.095	1.179	1.00	50.51
	118	CB	ILE	A	350	15.592	71.241	3.860	1.00	48.52
	119	CG1	ILE	A	350	15.172	71.562	5.299	1.00	49.25
	120	CG2	ILE	A	350	15.052	72.300	2.923	1.00	49.68
	121	CD1	ILE	A	350	13.689	71.358	5.567	1.00	46.80
15	122	N	ARG	A	351	17.021	69.335	2.155	1.00	52.64
	123	CA	ARG	A	351	17.807	68.931	1.000	1.00	53.76
	124	C	ARG	A	351	17.510	67.486	0.581	1.00	53.61
	125	O	ARG	A	351	17.506	67.164	-0.603	1.00	53.55
	126	CB	ARG	A	351	19.287	69.095	1.341	1.00	56.64
20	127	CG	ARG	A	351	20.166	69.584	0.206	1.00	62.18
	128	CD	ARG	A	351	21.225	70.527	0.752	1.00	66.96
	129	NE	ARG	A	351	22.389	70.642	-0.119	1.00	71.13
	130	CZ	ARG	A	351	23.229	69.643	-0.370	1.00	76.72
	131	NH1	ARG	A	351	23.027	68.455	0.184	1.00	78.73
25	132	NH2	ARG	A	351	24.275	69.829	-1.168	1.00	77.63
	133	N	LYS	A	352	17.253	66.626	1.560	1.00	53.86
	134	CA	LYS	A	352	16.954	65.215	1.312	1.00	54.12
	135	C	LYS	A	352	18.151	64.428	0.772	1.00	52.02
	136	O	LYS	A	352	17.996	63.522	-0.046	1.00	51.77
30	137	CB	LYS	A	352	15.775	65.075	0.347	1.00	57.77
	138	CG	LYS	A	352	14.476	65.689	0.846	1.00	62.15
	139	CD	LYS	A	352	13.348	65.439	-0.154	1.00	71.06
	140	CE	LYS	A	352	12.098	66.249	0.171	1.00	74.25
	141	NZ	LYS	A	352	12.293	67.707	-0.085	1.00	78.35
35	142	N	SER	A	353	19.342	64.789	1.233	1.00	48.01
	143	CA	SER	A	353	20.568	64.112	0.832	1.00	45.29
	144	C	SER	A	353	21.544	64.154	2.016	1.00	40.67
	145	O	SER	A	353	22.546	64.875	1.994	1.00	40.76
	146	CB	SER	A	353	21.177	64.791	-0.398	1.00	47.97
40	147	OG	SER	A	353	21.448	66.155	-0.147	1.00	56.20
	148	N	PRO	A	354	21.244	63.375	3.070	1.00	36.53
	149	CA	PRO	A	354	22.004	63.239	4.319	1.00	32.68
	150	C	PRO	A	354	23.399	62.660	4.139	1.00	31.88
	151	O	PRO	A	354	23.615	61.787	3.302	1.00	29.76
45	152	CB	PRO	A	354	21.147	62.294	5.160	1.00	30.29
	153	CG	PRO	A	354	19.799	62.340	4.513	1.00	41.68
	154	CD	PRO	A	354	20.106	62.445	3.065	1.00	33.29
	155	N	THR	A	355	24.342	63.154	4.932	1.00	30.03
	156	CA	THR	A	355	25.704	62.644	4.902	1.00	29.70
50	157	C	THR	A	355	26.236	62.578	6.326	1.00	30.82
	158	O	THR	A	355	25.773	63.298	7.213	1.00	30.67
	159	CB	THR	A	355	26.669	63.558	4.136	1.00	32.14
	160	OG1	THR	A	355	26.806	64.785	4.860	1.00	29.97
	161	CG2	THR	A	355	26.175	63.837	2.707	1.00	31.76
55	162	N	ILE	A	356	27.195	61.693	6.558	1.00	30.53
	163	CA	ILE	A	356	27.816	61.631	7.868	1.00	31.56
	164	C	ILE	A	356	29.279	61.860	7.575	1.00	31.79
	165	O	ILE	A	356	29.752	61.561	6.475	1.00	30.35
	166	CB	ILE	A	356	27.584	60.285	8.583	1.00	30.05
5	167	CG1	ILE	A	356	28.101	59.133	7.729	1.00	31.32
	168	CG2	ILE	A	356	26.093	60.131	8.890	1.00	31.27
	169	CD1	ILE	A	356	27.843	57.772	8.337	1.00	36.89
	170	N	THR	A	357	29.995	62.402	8.550	1.00	33.31
	171	CA	THR	A	357	31.395	62.719	8.349	1.00	33.68

	172	C	THR	A	357	32.282	62.197	9.456	1.00	35.47
	173	O	THR	A	357	31.993	62.372	10.641	1.00	36.65
	174	CB	THR	A	357	31.589	64.265	8.245	1.00	33.81
	175	OG1	THR	A	357	30.917	64.756	7.077	1.00	33.71
	176	CG2	THR	A	357	33.065	64.632	8.179	1.00	29.63
	177	N	CYS	A	358	33.372	61.566	9.052	1.00	35.41
	178	CA	CYS	A	358	34.346	61.039	9.990	1.00	38.12
	179	C	CYS	A	358	35.507	62.030	9.935	1.00	37.77
	180	O	CYS	A	358	36.127	62.205	8.890	1.00	36.67
	181	CB	CYS	A	358	34.811	59.655	9.532	1.00	40.37
	182	SG	CYS	A	358	35.831	58.729	10.726	1.00	49.83
	183	N	LEU	A	359	35.778	62.691	11.054	1.00	39.77
	184	CA	LEU	A	359	36.853	63.668	11.127	1.00	42.86
	185	C	LEU	A	359	38.007	63.168	11.977	1.00	46.01
	186	O	LEU	A	359	37.831	62.852	13.152	1.00	47.43
	187	CB	LEU	A	359	36.335	64.988	11.711	1.00	42.74
	188	CG	LEU	A	359	37.392	65.996	12.196	1.00	45.03
	189	CD1	LEU	A	359	38.262	66.448	11.043	1.00	47.59
	190	CD2	LEU	A	359	36.711	67.197	12.838	1.00	47.51
	191	N	VAL	A	360	39.189	63.107	11.379	1.00	48.26
	192	CA	VAL	A	360	40.380	62.669	12.090	1.00	52.34
	193	C	VAL	A	360	41.357	63.835	12.217	1.00	55.48
	194	O	VAL	A	360	41.672	64.508	11.234	1.00	55.57
	195	CB	VAL	A	360	41.073	61.500	11.353	1.00	53.36
	196	CG1	VAL	A	360	42.360	61.119	12.071	1.00	51.62
	197	CG2	VAL	A	360	40.133	60.301	11.284	1.00	51.77
	198	N	VAL	A	361	41.827	64.080	13.435	1.00	58.92
	199	CA	VAL	A	361	42.766	65.167	13.684	1.00	63.13
	200	C	VAL	A	361	44.094	64.607	14.174	1.00	67.77
	201	O	VAL	A	361	44.134	63.862	15.154	1.00	68.38
	202	CB	VAL	A	361	42.223	66.158	14.747	1.00	60.50
	203	CG1	VAL	A	361	43.245	67.242	15.014	1.00	56.92
	204	CG2	VAL	A	361	40.929	66.786	14.270	1.00	56.10
	205	N	ASP	A	362	45.174	64.965	13.485	1.00	72.90
	206	CA	ASP	A	362	46.515	64.502	13.841	1.00	78.30
	207	C	ASP	A	362	47.356	65.696	14.284	1.00	81.68
	208	O	ASP	A	362	47.891	66.432	13.452	1.00	81.72
	209	CB	ASP	A	362	47.185	63.829	12.638	1.00	80.22
	210	CG	ASP	A	362	48.444	63.070	13.020	1.00	84.67
	211	OD1	ASP	A	362	49.122	63.487	13.983	1.00	87.54
	212	OD2	ASP	A	362	48.763	62.063	12.351	1.00	87.19
	213	N	LEU	A	363	47.474	65.877	15.597	1.00	85.84
	214	CA	LEU	A	363	48.234	66.986	16.165	1.00	89.95
	215	C	LEU	A	363	49.677	67.038	15.672	1.00	92.20
	216	O	LEU	A	363	50.214	68.117	15.432	1.00	92.55
	217	CB	LEU	A	363	48.210	66.906	17.691	1.00	91.66
	218	CG	LEU	A	363	46.823	66.881	18.342	1.00	92.93
	219	CD1	LEU	A	363	46.976	66.787	19.854	1.00	95.41
	220	CD2	LEU	A	363	46.049	68.129	17.963	1.00	92.73
	221	N	ALA	A	364	50.304	65.874	15.527	1.00	94.76
	222	CA	ALA	A	364	51.684	65.799	15.049	1.00	97.66
	223	C	ALA	A	364	51.769	64.806	13.890	1.00	99.72
	224	O	ALA	A	364	51.604	63.602	14.079	1.00	100.44
	225	CB	ALA	A	364	52.604	65.365	16.179	1.00	97.99
	226	N	PRO	A	365	52.023	65.303	12.671	1.00	101.15
	227	CA	PRO	A	365	52.116	64.427	11.498	1.00	102.25
	228	C	PRO	A	365	53.437	63.705	11.245	1.00	103.43
	229	O	PRO	A	365	54.497	64.326	11.166	1.00	104.19
	230	CB	PRO	A	365	51.771	65.363	10.339	1.00	101.91
	231	CG	PRO	A	365	50.983	66.479	11.002	1.00	102.27
	232	CD	PRO	A	365	51.767	66.690	12.254	1.00	101.40
	233	N	SER	A	366	53.344	62.385	11.121	1.00	104.18

	234	CA	SER	A	366	54.468	61.512	10.801	1.00	104.43
	235	C	SER	A	366	53.924	61.027	9.463	1.00	104.05
	236	O	SER	A	366	52.736	60.712	9.373	1.00	104.36
	237	CB	SER	A	366	54.545	60.351	11.788	1.00	105.50
	238	OG	SER	A	366	53.377	59.560	11.687	1.00	106.70
	239	N	LYS	A	367	54.739	60.955	8.418	1.00	103.19
	240	CA	LYS	A	367	54.138	60.559	7.156	1.00	102.08
	241	C	LYS	A	367	53.970	59.109	6.733	1.00	100.74
	242	O	LYS	A	367	54.917	58.366	6.460	1.00	101.05
	243	CB	LYS	A	367	54.732	61.364	5.998	1.00	103.30
	244	CG	LYS	A	367	56.216	61.257	5.755	1.00	105.00
	245	CD	LYS	A	367	56.554	62.226	4.633	1.00	104.80
	246	CE	LYS	A	367	57.990	62.133	4.170	1.00	104.70
	247	NZ	LYS	A	367	58.214	63.076	3.034	1.00	105.18
	248	N	GLY	A	368	52.691	58.761	6.678	1.00	98.70
	249	CA	GLY	A	368	52.192	57.464	6.272	1.00	95.62
	250	C	GLY	A	368	50.799	57.900	5.856	1.00	93.12
	251	O	GLY	A	368	50.457	59.062	6.065	1.00	93.17
	252	N	THR	A	369	49.983	57.031	5.277	1.00	90.15
	253	CA	THR	A	369	48.652	57.475	4.880	1.00	86.41
	254	C	THR	A	369	47.623	57.180	5.964	1.00	83.04
	255	O	THR	A	369	47.746	56.198	6.699	1.00	82.54
	256	CB	THR	A	369	48.203	56.808	3.559	1.00	87.73
	257	OG1	THR	A	369	48.178	55.383	3.721	1.00	88.60
	258	CG2	THR	A	369	49.157	57.177	2.429	1.00	86.64
	259	N	VAL	A	370	46.620	58.048	6.073	1.00	79.07
	260	CA	VAL	A	370	45.559	57.871	7.058	1.00	74.46
	261	C	VAL	A	370	44.339	57.325	6.332	1.00	72.21
	262	O	VAL	A	370	43.762	57.998	5.482	1.00	71.35
	263	CB	VAL	A	370	45.180	59.199	7.732	1.00	73.33
	264	CG1	VAL	A	370	44.254	58.933	8.904	1.00	70.92
	265	CG2	VAL	A	370	46.427	59.926	8.185	1.00	69.77
	266	N	ASN	A	371	43.947	56.102	6.674	1.00	70.13
	267	CA	ASN	A	371	42.809	55.463	6.027	1.00	68.15
	268	C	ASN	A	371	41.521	55.443	6.838	1.00	65.65
	269	O	ASN	A	371	41.533	55.248	8.054	1.00	64.64
	270	CB	ASN	A	371	43.179	54.036	5.631	1.00	70.12
	271	CG	ASN	A	371	44.270	53.995	4.592	1.00	73.56
	272	OD1	ASN	A	371	44.081	54.447	3.462	1.00	75.10
	273	ND2	ASN	A	371	45.427	53.463	4.969	1.00	74.76
	274	N	LEU	A	372	40.408	55.651	6.141	1.00	62.66
	275	CA	LEU	A	372	39.088	55.641	6.754	1.00	59.53
	276	C	LEU	A	372	38.226	54.673	5.963	1.00	56.68
	277	O	LEU	A	372	38.071	54.812	4.753	1.00	56.70
	278	CB	LEU	A	372	38.459	57.040	6.728	1.00	59.44
	279	CG	LEU	A	372	39.217	58.172	7.422	1.00	60.55
	280	CD1	LEU	A	372	38.323	59.386	7.521	1.00	61.28
	281	CD2	LEU	A	372	39.644	57.739	8.807	1.00	62.83
	282	N	THR	A	373	37.669	53.689	6.654	1.00	53.76
	283	CA	THR	A	373	36.834	52.685	6.015	1.00	51.64
	284	C	THR	A	373	35.420	52.750	6.588	1.00	48.20
	285	O	THR	A	373	35.245	52.799	7.804	1.00	46.65
	286	CB	THR	A	373	37.399	51.275	6.268	1.00	53.15
	287	OG1	THR	A	373	38.811	51.276	6.027	1.00	57.77
	288	CG2	THR	A	373	36.729	50.261	5.353	1.00	53.75
	289	N	TRP	A	374	34.419	52.749	5.715	1.00	45.34
	290	CA	TRP	A	374	33.025	52.801	6.158	1.00	44.94
	291	C	TRP	A	374	32.341	51.439	6.059	1.00	43.68
	292	O	TRP	A	374	32.636	50.655	5.162	1.00	42.67
	293	CB	TRP	A	374	32.209	53.795	5.316	1.00	41.63
	294	CG	TRP	A	374	32.623	55.229	5.443	1.00	41.50
	295	CD1	TRP	A	374	33.476	55.912	4.623	1.00	39.67

	296	CD2	TRP	A	374	32.205	56.159	6.452	1.00	35.69
	297	NE1	TRP	A	374	33.612	57.208	5.059	1.00	35.06
	298	CE2	TRP	A	374	32.844	57.386	6.178	1.00	34.53
	299	CE3	TRP	A	374	31.353	56.072	7.558	1.00	32.37
	300	CZ2	TRP	A	374	32.657	58.521	6.971	1.00	35.43
	301	CZ3	TRP	A	374	31.166	57.199	8.349	1.00	36.11
	302	CH2	TRP	A	374	31.818	58.410	8.050	1.00	37.51
	303	N	SER	A	375	31.421	51.170	6.981	1.00	43.53
	304	CA	SER	A	375	30.666	49.922	6.960	1.00	43.57
	305	C	SER	A	375	29.330	50.089	7.662	1.00	42.59
	306	O	SER	A	375	29.189	50.931	8.550	1.00	43.68
	307	CB	SER	A	375	31.447	48.780	7.626	1.00	45.03
	308	OG	SER	A	375	31.482	48.909	9.034	1.00	45.66
	309	N	ARG	A	376	28.349	49.301	7.234	1.00	40.79
	310	CA	ARG	A	376	27.031	49.321	7.834	1.00	40.12
	311	C	ARG	A	376	26.911	48.102	8.749	1.00	40.59
	312	O	ARG	A	376	27.207	46.982	8.348	1.00	40.90
	313	CB	ARG	A	376	25.947	49.255	6.766	1.00	40.03
	314	CG	ARG	A	376	25.855	50.468	5.863	1.00	43.20
	315	CD	ARG	A	376	24.402	50.717	5.501	1.00	41.05
	316	NE	ARG	A	376	24.120	50.429	4.108	1.00	50.71
	317	CZ	ARG	A	376	22.895	50.300	3.612	1.00	53.97
	318	NH1	ARG	A	376	21.842	50.428	4.407	1.00	51.88
	319	NH2	ARG	A	376	22.726	50.058	2.318	1.00	55.55
	320	N	ALA	A	377	26.471	48.319	9.978	1.00	40.20
	321	CA	ALA	A	377	26.327	47.218	10.919	1.00	40.25
	322	C	ALA	A	377	25.470	46.100	10.314	1.00	40.38
	323	O	ALA	A	377	25.621	44.943	10.678	1.00	41.16
	324	CB	ALA	A	377	25.697	47.721	12.222	1.00	33.12
	325	N	SER	A	378	24.585	46.456	9.386	1.00	40.21
	326	CA	SER	A	378	23.697	45.491	8.746	1.00	41.95
	327	C	SER	A	378	24.412	44.694	7.664	1.00	44.92

	328	O	SER	A	378	23.856	43.734	7.134	1.00	44.28
	329	CB	SER	A	378	22.504	46.199	8.108	1.00	40.91
	330	OG	SER	A	378	22.907	46.863	6.920	1.00	40.09
	331	N	GLY	A	379	25.633	45.107	7.332	1.00	46.93
	332	CA	GLY	A	379	26.405	44.419	6.313	1.00	49.77
	333	C	GLY	A	379	26.088	44.884	4.904	1.00	50.60
	334	O	GLY	A	379	26.817	44.576	3.958	1.00	52.95
	335	N	LYS	A	380	24.995	45.626	4.755	1.00	53.72
	336	CA	LYS	A	380	24.612	46.122	3.443	1.00	54.13
	337	C	LYS	A	380	25.689	47.036	2.845	1.00	48.16
	338	O	LYS	A	380	26.592	47.513	3.544	1.00	45.65
	339	CB	LYS	A	380	23.262	46.848	3.517	1.00	62.44
	340	CG	LYS	A	380	22.078	45.908	3.710	1.00	67.72
	341	CD	LYS	A	380	20.748	46.625	3.550	1.00	69.32
	342	CE	LYS	A	380	19.587	45.644	3.619	1.00	73.14
	343	NZ	LYS	A	380	18.267	46.320	3.467	1.00	77.37
	344	N	PRO	A	381	25.614	47.277	1.529	1.00	56.07
	345	CA	PRO	A	381	26.586	48.128	0.835	1.00	56.46
	346	C	PRO	A	381	26.535	49.607	1.225	1.00	54.32
	347	O	PRO	A	381	25.467	50.154	1.511	1.00	56.76
	348	CB	PRO	A	381	26.225	47.936	-0.640	1.00	60.70
	349	CG	PRO	A	381	25.481	46.622	-0.667	1.00	62.01
	350	CD	PRO	A	381	24.655	46.695	0.574	1.00	59.24
	351	N	VAL	A	382	27.701	50.244	1.234	1.00	55.74
	352	CA	VAL	A	382	27.795	51.669	1.531	1.00	55.58
	353	C	VAL	A	382	28.192	52.353	0.220	1.00	55.56
	354	O	VAL	A	382	28.866	51.752	-0.620	1.00	55.22
	355	CB	VAL	A	382	28.874	51.980	2.607	1.00	55.39
	356	CG1	VAL	A	382	28.592	51.196	3.878	1.00	55.94
	357	CG2	VAL	A	382	30.261	51.664	2.075	1.00	53.06

	358	N	ASN	A	383	27.773	53.600	0.045	1.00	54.38
	359	CA	ASN	A	383	28.090	54.354	-1.164	1.00	54.63
	360	C	ASN	A	383	29.532	54.843	-1.190	1.00	53.85
	361	O	ASN	A	383	30.303	54.630	-0.254	1.00	52.58
	362	CB	ASN	A	383	27.171	55.566	-1.282	1.00	59.07
	363	CG	ASN	A	383	25.717	55.186	-1.356	1.00	64.60
	364	OD1	ASN	A	383	24.836	56.024	-1.169	1.00	70.14
	365	ND2	ASN	A	383	25.450	53.915	-1.638	1.00	71.07
	366	N	HIS	A	384	29.890	55.506	-2.281	1.00	53.46
	367	CA	HIS	A	384	31.229	56.057	-2.426	1.00	52.22
	368	C	HIS	A	384	31.326	57.302	-1.540	1.00	49.10
	369	O	HIS	A	384	30.400	58.105	-1.485	1.00	45.53
	370	CB	HIS	A	384	31.489	56.417	-3.893	1.00	59.11
	371	CG	HIS	A	384	31.676	55.223	-4.778	1.00	62.16
	372	ND1	HIS	A	384	32.738	54.357	-4.639	1.00	69.15
	373	CD2	HIS	A	384	30.931	54.745	-5.803	1.00	70.28
	374	CE1	HIS	A	384	32.640	53.394	-5.539	1.00	75.01
	375	NE2	HIS	A	384	31.553	53.605	-6.258	1.00	74.58
	376	N	SER	A	385	32.448	57.454	-0.849	1.00	45.07
	377	CA	SER	A	385	32.641	58.583	0.040	1.00	44.61
	378	C	SER	A	385	33.617	59.627	-0.504	1.00	44.58
	379	O	SER	A	385	34.380	59.356	-1.421	1.00	44.21
	380	CB	SER	A	385	33.113	58.076	1.409	1.00	44.61
	381	OG	SER	A	385	34.293	57.290	1.311	1.00	41.13
	382	N	THR	A	386	33.575	60.827	0.065	1.00	44.32
	383	CA	THR	A	386	34.450	61.916	-0.346	1.00	44.35
	384	C	THR	A	386	35.487	62.156	0.737	1.00	44.09
	385	O	THR	A	386	35.149	62.326	1.911	1.00	44.06
	386	CB	THR	A	386	33.664	63.226	-0.580	1.00	45.20
	387	OG1	THR	A	386	32.744	63.045	-1.662	1.00	51.89
	388	CG2	THR	A	386	34.616	64.368	-0.936	1.00	47.20
	389	N	ARG	A	387	36.749	62.176	0.326	1.00	44.39
	390	CA	ARG	A	387	37.870	62.378	1.233	1.00	46.68
	391	C	ARG	A	387	38.520	63.763	1.070	1.00	47.05
	392	O	ARG	A	387	38.750	64.228	-0.049	1.00	46.65
	393	CB	ARG	A	387	38.906	61.284	0.979	1.00	48.13
	394	CG	ARG	A	387	40.113	61.330	1.890	1.00	52.77
	395	CD	ARG	A	387	41.247	60.494	1.320	1.00	56.60
	396	NE	ARG	A	387	42.459	60.622	2.121	1.00	60.65
	397	CZ	ARG	A	387	42.705	59.917	3.218	1.00	61.97
	398	NH1	ARG	A	387	41.821	59.022	3.636	1.00	64.45
	399	NH2	ARG	A	387	43.819	60.131	3.911	1.00	60.54
	400	N	LYS	A	388	38.820	64.415	2.190	1.00	46.93
	401	CA	LYS	A	388	39.457	65.730	2.167	1.00	47.51
	402	C	LYS	A	388	40.630	65.777	3.143	1.00	48.33
	403	O	LYS	A	388	40.493	65.401	4.306	1.00	46.08
	404	CB	LYS	A	388	38.452	66.823	2.537	1.00	46.64
	405	CG	LYS	A	388	37.274	66.909	1.603	1.00	52.75
	406	CD	LYS	A	388	36.154	67.739	2.195	1.00	58.62
	407	CE	LYS	A	388	34.863	67.538	1.418	1.00	62.49
	408	NZ	LYS	A	388	33.719	68.204	2.101	1.00	67.33
	409	N	GLU	A	389	41.780	66.236	2.651	1.00	50.07
	410	CA	GLU	A	389	42.998	66.357	3.454	1.00	51.86
	411	C	GLU	A	389	43.474	67.807	3.462	1.00	52.81
	412	O	GLU	A	389	43.683	68.408	2.405	1.00	49.21
	413	CB	GLU	A	389	44.106	65.474	2.877	1.00	54.67
	414	CG	GLU	A	389	43.890	63.984	3.056	1.00	65.65
	415	CD	GLU	A	389	44.992	63.159	2.412	1.00	72.66
	416	OE1	GLU	A	389	46.182	63.449	2.671	1.00	75.92
	417	OE2	GLU	A	389	44.669	62.220	1.650	1.00	75.78
	418	N	GLU	A	390	43.652	68.371	4.651	1.00	56.06
	419	CA	GLU	A	390	44.100	69.751	4.754	1.00	61.17

	420	C	GLU	A	390	45.146	69.971	5.835	1.00	64.70
	421	O	GLU	A	390	45.002	69.528	6.977	1.00	64.01
	422	CB	GLU	A	390	42.908	70.673	4.993	1.00	64.35
	423	CG	GLU	A	390	43.283	72.121	5.233	1.00	74.80
	424	CD	GLU	A	390	42.091	73.052	5.121	1.00	85.97
	425	OE1	GLU	A	390	41.053	72.778	5.764	1.00	92.60
	426	OE2	GLU	A	390	42.197	74.059	4.388	1.00	92.18
	427	N	LYS	A	391	46.204	70.679	5.461	1.00	68.18
	428	CA	LYS	A	391	47.288	70.960	6.388	1.00	71.58
	429	C	LYS	A	391	47.298	72.385	6.920	1.00	76.11
	430	O	LYS	A	391	46.927	73.335	6.231	1.00	75.89
	431	CB	LYS	A	391	48.627	70.654	5.728	1.00	67.28
	432	N	GLN	A	392	47.724	72.508	8.168	1.00	81.85
	433	CA	GLN	A	392	47.854	73.786	8.846	1.00	88.38
	434	C	GLN	A	392	49.118	73.574	9.657	1.00	92.30
	435	O	GLN	A	392	49.100	72.848	10.648	1.00	93.25
	436	CB	GLN	A	392	46.662	74.045	9.777	1.00	85.87
	437	CG	GLN	A	392	45.752	75.178	9.318	1.00	90.76
	438	CD	GLN	A	392	44.727	75.573	10.369	1.00	93.39
	439	OE1	GLN	A	392	45.076	75.913	11.502	1.00	92.93
	440	NE2	GLN	A	392	43.453	75.538	9.993	1.00	93.97
	441	N	ARG	A	393	50.221	74.174	9.220	1.00	96.24
	442	CA	ARG	A	393	51.492	74.011	9.916	1.00	100.53
	443	C	ARG	A	393	51.412	74.350	11.403	1.00	102.30
	444	O	ARG	A	393	52.422	74.327	12.107	1.00	101.15
	445	CB	ARG	A	393	52.579	74.853	9.245	1.00	106.99
	446	CG	ARG	A	393	52.404	76.349	9.396	1.00	109.77
	447	CD	ARG	A	393	53.493	77.079	8.636	1.00	115.73
	448	NE	ARG	A	393	53.515	78.505	8.935	1.00	119.73
	449	CZ	ARG	A	393	54.333	79.373	8.350	1.00	121.60
	450	NH1	ARG	A	393	55.194	78.955	7.430	1.00	121.59
	451	NH2	ARG	A	393	54.292	80.655	8.684	1.00	121.49
	452	N	ASN	A	394	50.209	74.658	11.876	1.00	103.98
	453	CA	ASN	A	394	50.005	74.970	13.281	1.00	106.60
	454	C	ASN	A	394	50.275	73.682	14.051	1.00	106.89
	455	O	ASN	A	394	51.084	73.650	14.978	1.00	108.55
	456	CB	ASN	A	394	48.564	75.427	13.520	1.00	108.97
	457	CG	ASN	A	394	48.326	75.891	14.947	1.00	112.83
	458	OD1	ASN	A	394	47.190	76.141	15.348	1.00	114.53
	459	ND2	ASN	A	394	49.402	76.016	15.719	1.00	114.40
	460	N	GLY	A	395	49.593	72.616	13.648	1.00	105.53
	461	CA	GLY	A	395	49.771	71.331	14.298	1.00	101.15
	462	C	GLY	A	395	48.585	70.423	14.050	1.00	97.82
	463	O	GLY	A	395	48.125	69.721	14.952	1.00	99.41
	464	N	THR	A	396	48.084	70.423	12.822	1.00	94.50
	465	CA	THR	A	396	46.937	69.589	12.522	1.00	89.02
	466	C	THR	A	396	46.763	69.174	11.071	1.00	83.93
	467	O	THR	A	396	46.477	70.000	10.204	1.00	83.27
	468	CB	THR	A	396	45.625	70.278	12.970	1.00	92.03
	469	OG1	THR	A	396	45.648	70.484	14.388	1.00	94.17
	470	CG2	THR	A	396	44.414	69.421	12.596	1.00	95.48
	471	N	LEU	A	397	46.942	67.882	10.821	1.00	79.69
	472	CA	LEU	A	397	46.729	67.320	9.500	1.00	74.75
	473	C	LEU	A	397	45.295	66.827	9.604	1.00	71.50
	474	O	LEU	A	397	45.052	65.720	10.081	1.00	74.81
	475	CB	LEU	A	397	47.640	66.120	9.240	1.00	75.72
	476	CG	LEU	A	397	47.188	65.250	8.053	1.00	70.67
	477	CD1	LEU	A	397	47.668	65.858	6.738	1.00	69.05
	478	CD2	LEU	A	397	47.723	63.832	8.213	1.00	72.96
	479	N	THR	A	398	44.348	67.659	9.195	1.00	67.61
	480	CA	THR	A	398	42.945	67.286	9.252	1.00	61.30
	481	C	THR	A	398	42.559	66.393	8.076	1.00	56.61

	482	O	THR	A	398	42.960	66.626	6.934	1.00	54.95
	483	CB	THR	A	398	42.044	68.530	9.248	1.00	61.75
	484	OG1	THR	A	398	42.225	69.255	10.471	1.00	65.40
	485	CG2	THR	A	398	40.584	68.129	9.108	1.00	63.39
	486	N	VAL	A	399	41.783	65.359	8.371	1.00	51.84
	487	CA	VAL	A	399	41.321	64.437	7.349	1.00	48.05
	488	C	VAL	A	399	39.870	64.085	7.610	1.00	44.81
	489	O	VAL	A	399	39.502	63.689	8.719	1.00	44.41
	490	CB	VAL	A	399	42.132	63.134	7.349	1.00	49.35
	491	CG1	VAL	A	399	41.590	62.191	6.295	1.00	49.43
	492	CG2	VAL	A	399	43.594	63.432	7.090	1.00	53.10
	493	N	THR	A	400	39.036	64.246	6.596	1.00	42.44
	494	CA	THR	A	400	37.635	63.909	6.757	1.00	40.44
	495	C	THR	A	400	37.151	63.068	5.602	1.00	38.07
	496	O	THR	A	400	37.692	63.117	4.498	1.00	36.13
	497	CB	THR	A	400	36.731	65.152	6.834	1.00	39.64
	498	OG1	THR	A	400	36.638	65.755	5.539	1.00	43.72
	499	CG2	THR	A	400	37.278	66.158	7.822	1.00	38.32
	500	N	SER	A	401	36.140	62.265	5.884	1.00	36.90
	501	CA	SER	A	401	35.531	61.432	4.876	1.00	35.46
	502	C	SER	A	401	34.043	61.612	5.084	1.00	33.95
	503	O	SER	A	401	33.538	61.447	6.192	1.00	34.80
	504	CB	SER	A	401	35.906	59.962	5.060	1.00	36.91
	505	OG	SER	A	401	35.299	59.183	4.040	1.00	40.84
	506	N	THR	A	402	33.352	61.965	4.014	1.00	32.28
	507	CA	THR	A	402	31.928	62.178	4.068	1.00	31.85
	508	C	THR	A	402	31.245	61.092	3.264	1.00	31.76
	509	O	THR	A	402	31.554	60.863	2.090	1.00	30.55
	510	CB	THR	A	402	31.570	63.549	3.505	1.00	31.33
	511	OG1	THR	A	402	32.284	64.542	4.238	1.00	32.83
	512	CG2	THR	A	402	30.078	63.818	3.632	1.00	32.70
	513	N	LEU	A	403	30.299	60.433	3.912	1.00	30.72
	514	CA	LEU	A	403	29.582	59.343	3.300	1.00	30.33
	515	C	LEU	A	403	28.115	59.673	3.097	1.00	29.66
	516	O	LEU	A	403	27.415	59.992	4.052	1.00	28.06
	517	CB	LEU	A	403	29.698	58.098	4.187	1.00	28.34
	518	CG	LEU	A	403	28.968	56.831	3.719	1.00	32.10
	519	CD1	LEU	A	403	29.777	56.175	2.597	1.00	31.94
	520	CD2	LEU	A	403	28.810	55.844	4.876	1.00	30.42
	521	N	PRO	A	404	27.638	59.617	1.841	1.00	31.48
	522	CA	PRO	A	404	26.233	59.896	1.534	1.00	33.20
	523	C	PRO	A	404	25.451	58.759	2.194	1.00	34.02
	524	O	PRO	A	404	25.845	57.601	2.104	1.00	32.25
	525	CB	PRO	A	404	26.183	59.812	0.010	1.00	33.28
	526	CG	PRO	A	404	27.590	60.165	-0.400	1.00	31.82
	527	CD	PRO	A	404	28.413	59.414	0.603	1.00	31.26
	528	N	VAL	A	405	24.362	59.097	2.865	1.00	34.94
	529	CA	VAL	A	405	23.556	58.117	3.564	1.00	38.63
	530	C	VAL	A	405	22.128	58.059	3.032	1.00	40.02
	531	O	VAL	A	405	21.573	59.063	2.598	1.00	40.31
	532	CB	VAL	A	405	23.548	58.457	5.082	1.00	42.09
	533	CG1	VAL	A	405	22.128	58.490	5.632	1.00	43.95
	534	CG2	VAL	A	405	24.405	57.456	5.827	1.00	41.76
	535	N	GLY	A	406	21.536	56.872	3.061	1.00	42.35
	536	CA	GLY	A	406	20.168	56.741	2.597	1.00	43.35
	537	C	GLY	A	406	19.246	57.422	3.587	1.00	43.87
	538	O	GLY	A	406	19.446	57.314	4.797	1.00	42.68
	539	N	THR	A	407	18.248	58.134	3.077	1.00	44.40
	540	CA	THR	A	407	17.294	58.840	3.923	1.00	47.37
	541	C	THR	A	407	16.473	57.887	4.778	1.00	48.27
	542	O	THR	A	407	16.392	58.051	5.993	1.00	48.77
	543	CB	THR	A	407	16.312	59.678	3.078	1.00	48.44

	544	OG1	THR	A	407	17.001	60.791	2.504	1.00	50.00
	545	CG2	THR	A	407	15.164	60.187	3.938	1.00	53.23
	546	N	ARG	A	408	15.854	56.903	4.130	1.00	48.10
55	547	CA	ARG	A	408	15.021	55.935	4.821	1.00	48.54
	548	C	ARG	A	408	15.827	55.060	5.765	1.00	48.48
	549	O	ARG	A	408	15.418	54.831	6.903	1.00	47.34
	550	CB	ARG	A	408	14.275	55.070	3.810	1.00	50.16
	551	N	ASP	A	409	16.966	54.567	5.294	1.00	48.72
5	552	CA	ASP	A	409	17.813	53.714	6.121	1.00	50.88
	553	C	ASP	A	409	18.179	54.413	7.426	1.00	49.92
	554	O	ASP	A	409	18.132	53.811	8.502	1.00	49.76
	555	CB	ASP	A	409	19.088	53.340	5.362	1.00	56.18
	556	CG	ASP	A	409	18.799	52.587	4.074	1.00	64.80
10	557	OD1	ASP	A	409	18.118	51.538	4.144	1.00	71.41
	558	OD2	ASP	A	409	19.247	53.039	2.995	1.00	68.29
	559	N	TRP	A	410	18.533	55.692	7.327	1.00	48.36
	560	CA	TRP	A	410	18.914	56.458	8.503	1.00	46.32
	561	C	TRP	A	410	17.736	56.647	9.447	1.00	46.21
15	562	O	TRP	A	410	17.869	56.489	10.660	1.00	44.64
	563	CB	TRP	A	410	19.480	57.826	8.108	1.00	42.82
	564	CG	TRP	A	410	19.890	58.599	9.304	1.00	39.31
	565	CD1	TRP	A	410	19.133	59.496	9.997	1.00	37.29
	566	CD2	TRP	A	410	21.093	58.419	10.057	1.00	35.49
20	567	NE1	TRP	A	410	19.781	59.874	11.143	1.00	39.24
	568	CE2	TRP	A	410	20.987	59.228	11.205	1.00	32.76
	569	CE3	TRP	A	410	22.249	57.644	9.872	1.00	32.07
	570	CZ2	TRP	A	410	21.994	59.291	12.176	1.00	29.59
	571	CZ3	TRP	A	410	23.248	57.704	10.831	1.00	33.68
25	572	CH2	TRP	A	410	23.111	58.527	11.975	1.00	30.56
	573	N	ILE	A	411	16.584	56.989	8.888	1.00	48.11
	574	CA	ILE	A	411	15.391	57.192	9.699	1.00	50.90
	575	C	ILE	A	411	14.951	55.888	10.358	1.00	52.46
	576	O	ILE	A	411	14.371	55.902	11.442	1.00	53.34
30	577	CB	ILE	A	411	14.234	57.755	8.854	1.00	51.58
	578	CG1	ILE	A	411	14.613	59.144	8.330	1.00	52.81
	579	CG2	ILE	A	411	12.966	57.828	9.685	1.00	51.95
	580	CD1	ILE	A	411	13.566	59.777	7.431	1.00	59.38
	581	N	GLU	A	412	15.252	54.763	9.715	1.00	53.21
35	582	CA	GLU	A	412	14.872	53.463	10.248	1.00	53.12
	583	C	GLU	A	412	15.853	52.919	11.269	1.00	51.24
	584	O	GLU	A	412	15.610	51.864	11.848	1.00	51.40
	585	CB	GLU	A	412	14.691	52.448	9.119	1.00	59.71
	586	CG	GLU	A	412	13.362	52.578	8.383	1.00	70.52
40	587	CD	GLU	A	412	13.201	51.540	7.290	1.00	78.58
	588	OE1	GLU	A	412	13.402	50.338	7.573	1.00	83.44
	589	OE2	GLU	A	412	12.868	51.924	6.150	1.00	82.10
	590	N	GLY	A	413	16.966	53.618	11.477	1.00	48.47
	591	CA	GLY	A	413	17.923	53.173	12.474	1.00	44.62
45	592	C	GLY	A	413	19.213	52.484	12.068	1.00	44.15
	593	O	GLY	A	413	19.882	51.913	12.927	1.00	43.50
	594	N	GLU	A	414	19.588	52.515	10.793	1.00	42.78
	595	CA	GLU	A	414	20.843	51.878	10.406	1.00	40.78
	596	C	GLU	A	414	21.948	52.495	11.249	1.00	39.97
50	597	O	GLU	A	414	21.842	53.645	11.690	1.00	37.43
	598	CB	GLU	A	414	21.155	52.111	8.918	1.00	41.96
	599	CG	GLU	A	414	22.519	51.566	8.441	1.00	44.09
	600	CD	GLU	A	414	22.582	50.036	8.360	1.00	49.01
	601	OE1	GLU	A	414	23.051	49.387	9.325	1.00	46.84
55	602	OE2	GLU	A	414	22.152	49.479	7.327	1.00	49.89

603	N	THR	A	415	23.001	51.721	11.485	1.00	39.56
604	CA	THR	A	415	24.136	52.197	12.253	1.00	40.76
605	C	THR	A	415	25.369	52.113	11.362	1.00	40.07
606	O	THR	A	415	25.640	51.067	10.777	1.00	42.10
607	CB	THR	A	415	24.327	51.362	13.544	1.00	44.69
608	OG1	THR	A	415	25.707	51.378	13.929	1.00	51.98
609	CG2	THR	A	415	23.856	49.948	13.342	1.00	50.00
610	N	TYR	A	416	26.100	53.220	11.240	1.00	37.57
611	CA	TYR	A	416	27.282	53.273	10.386	1.00	34.50
612	C	TYR	A	416	28.549	53.335	11.201	1.00	36.77
613	O	TYR	A	416	28.562	53.894	12.300	1.00	35.94
614	CB	TYR	A	416	27.221	54.484	9.466	1.00	34.15
615	CG	TYR	A	416	26.003	54.515	8.586	1.00	30.65
616	CD1	TYR	A	416	24.744	54.823	9.108	1.00	32.53
617	CD2	TYR	A	416	26.101	54.211	7.235	1.00	31.72
618	CE1	TYR	A	416	23.616	54.828	8.297	1.00	34.27
619	CE2	TYR	A	416	24.981	54.210	6.420	1.00	32.11
620	CZ	TYR	A	416	23.744	54.520	6.956	1.00	33.86
621	OH	TYR	A	416	22.636	54.518	6.139	1.00	41.22
622	N	GLN	A	417	29.624	52.771	10.659	1.00	37.58
623	CA	GLN	A	417	30.878	52.752	11.386	1.00	39.43
624	C	GLN	A	417	32.062	53.259	10.582	1.00	39.40
625	O	GLN	A	417	32.227	52.936	9.406	1.00	39.63
626	CB	GLN	A	417	31.179	51.331	11.889	1.00	41.37
627	CG	GLN	A	417	32.386	51.250	12.822	1.00	51.81
628	CD	GLN	A	417	32.744	49.827	13.214	1.00	61.69
629	OE1	GLN	A	417	33.229	49.045	12.390	1.00	67.15
630	NE2	GLN	A	417	32.504	49.481	14.479	1.00	63.64
631	N	CYS	A	418	33.888	54.057	11.236	1.00	39.29
632	CA	CYS	A	418	34.083	54.581	10.611	1.00	41.80
633	C	CYS	A	418	35.250	53.880	11.282	1.00	42.50
634	O	CYS	A	418	35.409	53.954	12.500	1.00	43.33
635	CB	CYS	A	418	34.208	56.099	10.825	1.00	41.95
636	SG	CYS	A	418	35.696	56.805	10.043	1.00	54.15
637	N	ARG	A	419	36.049	53.182	10.491	1.00	43.98
638	CA	ARG	A	419	37.225	52.497	11.007	1.00	47.51
639	C	ARG	A	419	38.428	53.323	10.558	1.00	48.11
640	O	ARG	A	419	38.741	53.381	9.370	1.00	47.85
641	CB	ARG	A	419	37.289	51.068	10.452	1.00	49.08
642	CG	ARG	A	419	38.642	50.397	10.586	1.00	54.11
643	CD	ARG	A	419	38.554	48.892	10.304	1.00	64.71
644	NE	ARG	A	419	39.868	48.275	10.137	1.00	64.09
645	CZ	ARG	A	419	40.493	48.163	8.968	1.00	70.31
646	NH1	ARG	A	419	39.919	48.619	7.861	1.00	68.32
647	NH2	ARG	A	419	41.699	47.608	8.905	1.00	71.53
648	N	VAL	A	420	39.076	53.990	11.508	1.00	51.04
649	CA	VAL	A	420	40.231	54.824	11.200	1.00	56.22
650	C	VAL	A	420	41.532	54.039	11.354	1.00	61.25
651	O	VAL	A	420	41.780	53.422	12.393	1.00	60.11
652	CB	VAL	A	420	40.295	56.064	12.115	1.00	54.44
653	CG1	VAL	A	420	41.494	56.922	11.729	1.00	52.69
654	CG2	VAL	A	420	39.003	56.868	12.005	1.00	55.45
655	N	THR	A	421	42.359	54.071	10.314	1.00	66.23
656	CA	THR	A	421	43.631	53.356	10.326	1.00	73.18
657	C	THR	A	421	44.834	54.266	10.130	1.00	76.87
658	O	THR	A	421	45.157	54.632	9.000	1.00	77.93
659	CB	THR	A	421	43.671	52.283	9.225	1.00	73.75
660	OG1	THR	A	421	42.628	51.328	9.451	1.00	77.71
661	CG2	THR	A	421	45.009	51.567	9.227	1.00	75.35
662	N	HIS	A	422	45.499	54.624	11.226	1.00	81.02
663	CA	HIS	A	422	46.678	55.483	11.151	1.00	86.07

664	C	HIS	A	422	47.914	54.596	11.278	1.00	89.67
665	O	HIS	A	422	47.947	53.680	12.098	1.00	90.00
666	CB	HIS	A	422	46.660	56.529	12.269	1.00	87.43
667	CG	HIS	A	422	47.548	57.708	12.008	1.00	90.73
668	ND1	HIS	A	422	47.397	58.524	10.909	1.00	93.83
669	CD2	HIS	A	422	48.600	58.204	12.704	1.00	91.89
670	CE1	HIS	A	422	48.318	59.473	10.936	1.00	94.70
671	NE2	HIS	A	422	49.060	59.300	12.015	1.00	93.25
672	N	PRO	A	423	48.954	54.871	10.474	1.00	92.64
673	CA	PRO	A	423	50.209	54.111	10.460	1.00	95.19
674	C	PRO	A	423	50.838	53.628	11.775	1.00	97.06
675	O	PRO	A	423	51.064	52.431	11.945	1.00	97.57
676	CB	PRO	A	423	51.155	55.024	9.667	1.00	95.56
677	CG	PRO	A	423	50.566	56.391	9.853	1.00	93.94
678	CD	PRO	A	423	49.105	56.112	9.696	1.00	93.12
679	N	HIS	A	424	51.105	54.542	12.701	1.00	98.71
680	CA	HIS	A	424	51.769	54.190	13.957	1.00	100.16
681	C	HIS	A	424	51.021	53.496	15.095	1.00	99.67
682	O	HIS	A	424	51.609	52.690	15.816	1.00	99.61
683	CB	HIS	A	424	52.451	55.435	14.522	1.00	102.42
684	CG	HIS	A	424	53.475	56.022	13.605	1.00	105.47
685	ND1	HIS	A	424	53.372	57.298	13.092	1.00	107.10
686	CD2	HIS	A	424	54.639	55.521	13.133	1.00	97.46
687	CE1	HIS	A	424	54.430	57.556	12.345	1.00	106.81
688	NE2	HIS	A	424	55.215	56.494	12.353	1.00	106.61
689	N	LEU	A	425	49.742	53.798	15.267	1.00	99.19
690	CA	LEU	A	425	48.972	53.216	16.363	1.00	99.01
691	C	LEU	A	425	48.692	51.714	16.284	1.00	98.36
692	O	LEU	A	425	48.479	51.160	15.204	1.00	98.39
693	CB	LEU	A	425	47.671	53.994	16.507	1.00	100.66
694	CG	LEU	A	425	47.969	55.495	16.467	1.00	101.95
695	CD1	LEU	A	425	46.683	56.285	16.569	1.00	102.59
696	CD2	LEU	A	425	48.923	55.856	17.598	1.00	103.85
697	N	PRO	A	426	48.685	51.038	17.448	1.00	97.57
698	CA	PRO	A	426	48.435	49.596	17.540	1.00	96.82
699	C	PRO	A	426	47.075	49.186	16.992	1.00	95.53
700	O	PRO	A	426	46.990	48.560	15.937	1.00	95.77
701	CB	PRO	A	426	48.570	49.318	19.037	1.00	97.13
702	CG	PRO	A	426	48.106	50.605	19.660	1.00	97.88
703	CD	PRO	A	426	48.802	51.631	18.793	1.00	97.70
704	N	ARG	A	427	46.015	49.536	17.713	1.00	94.16
705	CA	ARG	A	427	44.669	49.198	17.274	1.00	92.52
706	C	ARG	A	427	44.091	50.315	16.408	1.00	89.85
707	O	ARG	A	427	44.487	51.477	16.517	1.00	89.26
708	CB	ARG	A	427	43.749	48.948	18.478	1.00	97.34
709	CG	ARG	A	427	42.381	48.398	18.077	1.00	99.32
710	CD	ARG	A	427	41.428	48.193	19.253	1.00	105.99
711	NE	ARG	A	427	40.197	47.532	18.815	1.00	111.10
712	CZ	ARG	A	427	39.140	47.298	19.588	1.00	111.66
713	NH1	ARG	A	427	39.143	47.673	20.861	1.00	111.70
714	NH2	ARG	A	427	38.078	46.679	19.087	1.00	110.09
715	N	ALA	A	428	43.158	49.949	15.538	1.00	86.56
716	CA	ALA	A	428	42.513	50.910	14.661	1.00	82.70
717	C	ALA	A	428	41.389	51.602	15.423	1.00	80.03
718	O	ALA	A	428	40.711	50.981	16.239	1.00	80.29
719	CB	ALA	A	428	41.953	50.200	13.437	1.00	83.85
720	N	LEU	A	429	41.203	52.892	15.164	1.00	76.76
721	CA	LEU	A	429	40.144	53.651	15.815	1.00	72.72
722	C	LEU	A	429	38.820	53.289	15.164	1.00	69.67
723	O	LEU	A	429	38.742	53.128	13.947	1.00	68.64
724	CB	LEU	A	429	40.392	55.156	15.671	1.00	73.60
725	CG	LEU	A	429	41.169	55.847	16.793	1.00	73.35

	726	CD1	LEU	A	429	41.498	57.280	16.404	1.00	72.09
	727	CD2	LEU	A	429	40.333	55.813	18.065	1.00	76.40
	728	N	MET	A	430	37.779	53.153	15.976	1.00	66.83
	729	CA	MET	A	430	36.468	52.814	15.449	1.00	64.81
	730	C	MET	A	430	35.384	53.678	16.074	1.00	61.41
	731	O	MET	A	430	35.274	53.776	17.299	1.00	60.84
	732	CB	MET	A	430	36.173	51.335	15.691	1.00	68.22
	733	CG	MET	A	430	37.247	50.416	15.133	1.00	74.39
	734	SD	MET	A	430	36.886	48.679	15.387	1.00	83.18
	735	CE	MET	A	430	36.836	48.607	17.194	1.00	84.12
	736	N	ARG	A	431	34.590	54.312	15.218	1.00	57.17
	737	CA	ARG	A	431	33.506	55.172	15.674	1.00	54.04
	738	C	ARG	A	431	32.234	54.752	14.963	1.00	50.58
	739	O	ARG	A	431	32.270	54.367	13.796	1.00	50.46
	740	CB	ARG	A	431	33.825	56.641	15.364	1.00	55.16
	741	CG	ARG	A	431	35.036	57.187	16.109	1.00	59.24
	742	CD	ARG	A	431	34.802	57.172	17.611	1.00	63.93
	743	NE	ARG	A	431	35.983	57.586	18.363	1.00	70.30
	744	CZ	ARG	A	431	36.070	57.557	19.689	1.00	76.24
	745	NH1	ARG	A	431	35.041	57.131	20.417	1.00	77.83
	746	NH2	ARG	A	431	37.185	57.952	20.289	1.00	77.12
	747	N	SER	A	432	31.112	54.812	15.669	1.00	46.92
	748	CA	SER	A	432	29.835	54.437	15.084	1.00	45.15
	749	C	SER	A	432	28.784	55.482	15.398	1.00	42.49
	750	O	SER	A	432	28.901	56.218	16.379	1.00	42.76
	751	CB	SER	A	432	29.394	53.068	15.610	1.00	44.31
	752	OG	SER	A	432	29.316	53.084	17.018	1.00	49.96
	753	N	THR	A	433	27.749	55.540	14.570	1.00	40.28
	754	CA	THR	A	433	26.691	56.522	14.763	1.00	39.71
	755	C	THR	A	433	25.356	55.996	14.257	1.00	39.49
	756	O	THR	A	433	25.315	55.186	13.334	1.00	40.22
	757	CB	THR	A	433	27.023	57.839	14.022	1.00	38.07
	758	OG1	THR	A	433	26.006	58.807	14.295	1.00	39.56
	759	CG2	THR	A	433	27.088	57.609	12.518	1.00	36.99
	760	N	THR	A	434	24.272	56.461	14.874	1.00	39.18
	761	CA	THR	A	434	22.913	56.068	14.512	1.00	40.70
	762	C	THR	A	434	21.965	57.186	14.934	1.00	40.23
	763	O	THR	A	434	22.364	58.091	15.659	1.00	41.18
	764	CB	THR	A	434	22.484	54.784	15.256	1.00	43.01
	765	OG1	THR	A	434	22.362	55.052	16.661	1.00	47.85
	766	CG2	THR	A	434	23.524	53.726	15.105	1.00	48.67
	767	N	LYS	A	435	20.714	57.125	14.496	1.00	40.97
	768	CA	LYS	A	435	19.767	58.150	14.889	1.00	45.73
	769	C	LYS	A	435	19.601	58.021	16.398	1.00	48.93
	770	O	LYS	A	435	19.710	56.930	16.942	1.00	48.49
	771	CB	LYS	A	435	18.434	57.937	14.194	1.00	45.94
	772	N	THR	A	436	19.365	59.133	17.082	1.00	52.01
	773	CA	THR	A	436	19.171	59.080	18.526	1.00	54.88
	774	C	THR	A	436	17.722	58.684	18.774	1.00	55.70
	775	O	THR	A	436	16.823	59.146	18.077	1.00	55.21
	776	CB	THR	A	436	19.438	60.454	19.191	1.00	56.24
	777	OG1	THR	A	436	20.821	60.802	19.038	1.00	60.56
	778	CG2	THR	A	436	19.090	60.412	20.677	1.00	57.04
	779	N	SER	A	437	17.501	57.810	19.748	1.00	57.93
	780	CA	SER	A	437	16.149	57.380	20.080	1.00	60.42
	781	C	SER	A	437	15.683	58.239	21.249	1.00	60.49
	782	O	SER	A	437	16.357	59.203	21.623	1.00	60.21
	783	CB	SER	A	437	16.133	55.894	20.470	1.00	61.57
	784	OG	SER	A	437	16.957	55.651	21.600	1.00	65.51
	785	N	GLY	A	438	14.533	57.895	21.821	1.00	60.09
	786	CA	GLY	A	438	14.022	58.666	22.939	1.00	58.42
	787	C	GLY	A	438	12.937	59.630	22.511	1.00	57.80

	788	O	GLY	A	438	12.648	59.747	21.322	1.00	56.51
	789	N	PRO	A	439	12.309	60.333	23.467	1.00	57.81
	790	CA	PRO	A	439	11.242	61.295	23.185	1.00	56.19
	791	C	PRO	A	439	11.692	62.422	22.263	1.00	53.91
	792	O	PRO	A	439	12.886	62.709	22.147	1.00	53.91
	793	CB	PRO	A	439	10.865	61.806	24.576	1.00	57.79
	794	CG	PRO	A	439	11.147	60.633	25.448	1.00	58.60
	795	CD	PRO	A	439	12.485	60.173	24.921	1.00	60.65
	796	N	ARG	A	440	10.722	63.055	21.612	1.00	51.09
	797	CA	ARG	A	440	10.990	64.163	20.702	1.00	48.90
	798	C	ARG	A	440	10.220	65.365	21.231	1.00	45.83
	799	O	ARG	A	440	9.188	65.202	21.881	1.00	45.88
	800	CB	ARG	A	440	10.501	63.836	19.289	1.00	49.95
	801	CG	ARG	A	440	10.919	62.473	18.771	1.00	59.03
	802	CD	ARG	A	440	12.406	62.373	18.448	1.00	65.31
	803	NE	ARG	A	440	12.814	60.973	18.342	1.00	72.31
	804	CZ	ARG	A	440	13.986	60.553	17.878	1.00	74.99
	805	NH1	ARG	A	440	14.894	61.419	17.460	1.00	77.22
	806	NH2	ARG	A	440	14.252	59.255	17.837	1.00	78.59
	807	N	ALA	A	441	10.727	66.564	20.957	1.00	42.09
	808	CA	ALA	A	441	10.079	67.800	21.387	1.00	39.26
	809	C	ALA	A	441	10.476	68.894	20.413	1.00	38.22
	810	O	ALA	A	441	11.649	69.034	20.076	1.00	38.95
	811	CB	ALA	A	441	10.511	68.170	22.798	1.00	36.56
	812	N	ALA	A	442	9.496	69.666	19.966	1.00	37.22
	813	CA	ALA	A	442	9.739	70.729	19.011	1.00	37.60
	814	C	ALA	A	442	10.550	71.879	19.590	1.00	38.65
	815	O	ALA	A	442	10.553	72.103	20.798	1.00	40.22
	816	CB	ALA	A	442	8.415	71.248	18.481	1.00	37.17
	817	N	PRO	A	443	11.260	72.619	18.722	1.00	38.04
	818	CA	PRO	A	443	12.089	73.765	19.104	1.00	36.79
	819	C	PRO	A	443	11.224	75.019	19.243	1.00	38.14
	820	O	PRO	A	443	10.236	75.174	18.521	1.00	37.39
	821	CB	PRO	A	443	13.050	73.923	17.921	1.00	36.30
	822	CG	PRO	A	443	12.946	72.632	17.159	1.00	36.35
	823	CD	PRO	A	443	11.512	72.249	17.320	1.00	37.85
	824	N	GLU	A	444	11.594	75.894	20.173	1.00	36.28
	825	CA	GLU	A	444	10.901	77.163	20.371	1.00	35.57
	826	C	GLU	A	444	11.941	78.171	19.888	1.00	33.87
	827	O	GLU	A	444	13.110	78.105	20.291	1.00	33.43
	828	CB	GLU	A	444	10.580	77.383	21.851	1.00	38.68
	829	N	VAL	A	445	11.520	79.097	19.033	1.00	30.18
	830	CA	VAL	A	445	12.432	80.070	18.450	1.00	28.24
	831	C	VAL	A	445	12.136	81.523	18.811	1.00	28.44
	832	O	VAL	A	445	11.000	81.975	18.721	1.00	26.78
	833	CB	VAL	A	445	12.417	79.937	16.905	1.00	28.10
	834	CG1	VAL	A	445	13.370	80.933	16.274	1.00	25.56
	835	CG2	VAL	A	445	12.771	78.521	16.511	1.00	26.30
	836	N	TYR	A	446	13.175	82.251	19.203	1.00	27.87
	837	CA	TYR	A	446	13.019	83.651	19.551	1.00	27.91
	838	C	TYR	A	446	14.193	84.460	19.024	1.00	27.06
	839	O	TYR	A	446	15.326	84.307	19.480	1.00	27.96
	840	CB	TYR	A	446	12.898	83.836	21.074	1.00	26.45
	841	CG	TYR	A	446	12.749	85.289	21.447	1.00	26.59
	842	CD1	TYR	A	446	11.714	86.057	20.905	1.00	28.48
	843	CD2	TYR	A	446	13.659	85.914	22.305	1.00	29.02
	844	CE1	TYR	A	446	11.589	87.417	21.204	1.00	33.24
	845	CE2	TYR	A	446	13.543	87.274	22.616	1.00	31.33
	846	CZ	TYR	A	446	12.506	88.015	22.059	1.00	36.01
	847	OH	TYR	A	446	12.387	89.352	22.338	1.00	36.54
	848	N	ALA	A	447	13.914	85.326	18.060	1.00	28.07
	849	CA	ALA	A	447	14.949	86.150	17.439	1.00	27.67

	850	C	ALA	A	447	14.815	87.579	17.932	1.00	29.19
	851	O	ALA	A	447	13.702	88.036	18.173	1.00	31.10
	852	CB	ALA	A	447	14.802	86.098	15.931	1.00	23.97
	853	N	PHE	A	448	15.929	88.293	18.079	1.00	29.56
	854	CA	PHE	A	448	15.849	89.657	18.578	1.00	32.50
	855	C	PHE	A	448	17.075	90.483	18.246	1.00	33.67
	856	O	PHE	A	448	18.112	89.950	17.872	1.00	35.26
	857	CB	PHE	A	448	15.659	89.630	20.097	1.00	35.29
	858	CG	PHE	A	448	16.849	89.077	20.838	1.00	37.04
	859	CD1	PHE	A	448	17.912	89.909	21.195	1.00	36.66
	860	CD2	PHE	A	448	16.934	87.714	21.127	1.00	34.95
	861	CE1	PHE	A	448	19.049	89.382	21.824	1.00	40.91
	862	CE2	PHE	A	448	18.066	87.178	21.753	1.00	35.99
	863	CZ	PHE	A	448	19.123	88.014	22.103	1.00	35.15
	864	N	ALA	A	449	16.952	91.796	18.396	1.00	35.81
	865	CA	ALA	A	449	18.066	92.693	18.131	1.00	37.63
	866	C	ALA	A	449	18.617	93.253	19.438	1.00	40.96
	867	O	ALA	A	449	17.885	93.441	20.403	1.00	40.14
	868	CB	ALA	A	449	17.623	93.831	17.230	1.00	33.60
	869	N	THR	A	450	19.918	93.509	19.448	1.00	45.40
	870	CA	THR	A	450	20.606	94.071	20.595	1.00	50.82
	871	C	THR	A	450	20.515	95.597	20.498	1.00	53.78
	872	O	THR	A	450	20.673	96.169	19.417	1.00	54.14
	873	CB	THR	A	450	22.090	93.665	20.587	1.00	51.45
	874	OG1	THR	A	450	22.192	92.242	20.450	1.00	54.12
	875	CG2	THR	A	450	22.769	94.093	21.877	1.00	55.58
	876	N	PRO	A	451	20.260	96.275	21.626	1.00	56.74
	877	CA	PRO	A	451	20.157	97.737	21.623	1.00	59.05
	878	C	PRO	A	451	21.427	98.391	21.080	1.00	61.00
	879	O	PRO	A	451	22.535	98.080	21.521	1.00	59.71
	880	CB	PRO	A	451	19.933	98.073	23.098	1.00	60.52
	881	CG	PRO	A	451	19.262	96.851	23.640	1.00	61.14
	882	CD	PRO	A	451	20.049	95.739	22.981	1.00	59.39
	883	N	GLU	A	452	21.272	99.285	20.112	1.00	64.30
	884	CA	GLU	A	452	22.428	99.975	19.558	1.00	69.17
	885	C	GLU	A	452	22.252	101.463	19.842	1.00	72.61
	886	O	GLU	A	452	21.667	102.206	19.057	1.00	73.59
	887	CB	GLU	A	452	22.560	99.712	18.054	1.00	65.66
	888	CG	GLU	A	452	24.015	99.566	17.577	1.00	61.46
	889	CD	GLU	A	452	24.717	98.317	18.133	1.00	60.52
	890	OE1	GLU	A	452	24.053	97.264	18.251	1.00	63.47
	891	OE2	GLU	A	452	25.934	98.373	18.433	1.00	53.34
	892	N	TRP	A	453	22.763	101.869	20.997	1.00	76.75
	893	CA	TRP	A	453	22.693	103.242	21.481	1.00	81.00
	894	C	TRP	A	453	23.886	104.027	20.913	1.00	82.30
	895	O	TRP	A	453	25.038	103.710	21.215	1.00	82.08
	896	CB	TRP	A	453	22.737	103.191	23.010	1.00	85.65
	897	CG	TRP	A	453	22.182	104.367	23.734	1.00	89.76
	898	CD1	TRP	A	453	20.939	104.921	23.588	1.00	92.34
	899	CD2	TRP	A	453	22.819	105.083	24.795	1.00	94.15
	900	NE1	TRP	A	453	20.764	105.934	24.502	1.00	94.99
	901	CE2	TRP	A	453	21.904	106.055	25.255	1.00	95.56
	902	CE3	TRP	A	453	24.079	104.995	25.407	1.00	95.36
	903	CZ2	TRP	A	453	22.208	106.935	26.300	1.00	97.14
	904	CZ3	TRP	A	453	24.380	105.869	26.445	1.00	95.61
	905	CH2	TRP	A	453	23.447	106.826	26.880	1.00	97.12
	906	N	PRO	A	454	23.619	105.058	20.080	1.00	84.10
	907	CA	PRO	A	454	24.606	105.931	19.422	1.00	87.24
	908	C	PRO	A	454	25.892	106.316	20.162	1.00	90.52
	909	O	PRO	A	454	26.088	105.978	21.333	1.00	89.75
	910	CB	PRO	A	454	23.775	107.150	18.988	1.00	84.91
	911	CG	PRO	A	454	22.475	107.017	19.740	1.00	83.62

	912	CD	PRO	A	454	22.259	105.537	19.793	1.00	84.60
	913	N	GLY	A	455	26.751	107.055	19.464	1.00	91.72
	914	CA	GLY	A	455	28.048	107.413	20.012	1.00	94.13
	915	C	GLY	A	455	28.730	106.132	19.601	1.00	96.28
	916	O	GLY	A	455	28.613	105.125	20.301	1.00	97.74
	917	N	SER	A	456	29.442	106.142	18.478	1.00	99.11
	918	CA	SER	A	456	29.974	104.869	18.023	1.00	96.15
	919	C	SER	A	456	31.407	104.465	17.676	1.00	91.50
	920	O	SER	A	456	32.292	105.284	17.333	1.00	88.52
	921	CB	SER	A	456	29.092	104.378	16.879	1.00	95.05
	922	OG	SER	A	456	28.910	105.375	15.884	1.00	110.76
	923	N	ARG	A	457	31.541	103.136	17.752	1.00	87.73
	924	CA	ARG	A	457	32.664	102.251	17.520	1.00	87.81
	925	C	ARG	A	457	31.678	101.103	17.647	1.00	86.30
	926	O	ARG	A	457	31.026	100.998	18.697	1.00	90.57
	927	CB	ARG	A	457	33.634	102.261	18.675	1.00	94.67
	928	N	ASP	A	458	31.512	100.259	16.627	1.00	87.32
	929	CA	ASP	A	458	30.441	99.286	16.780	1.00	80.43
	930	C	ASP	A	458	30.422	97.963	16.080	1.00	72.83
	931	O	ASP	A	458	31.410	97.437	15.599	1.00	73.96
	932	CB	ASP	A	458	29.150	99.985	16.385	1.00	83.19
	933	CG	ASP	A	458	29.102	100.300	14.890	1.00	85.09
	934	OD1	ASP	A	458	30.065	100.906	14.378	1.00	91.25
	935	OD2	ASP	A	458	28.108	99.939	14.217	1.00	90.84
	936	N	LYS	A	459	29.196	97.451	16.076	1.00	66.05
	937	CA	LYS	A	459	28.782	96.211	15.437	1.00	61.75
	938	C	LYS	A	459	27.368	95.983	15.886	1.00	56.14
	939	O	LYS	A	459	27.144	95.648	17.046	1.00	56.54
	940	CB	LYS	A	459	29.641	95.031	15.889	1.00	68.18
	941	CG	LYS	A	459	30.801	94.804	14.969	1.00	71.85
	942	CD	LYS	A	459	30.406	94.863	13.499	1.00	73.79
	943	CE	LYS	A	459	31.655	94.839	12.626	1.00	76.14
	944	NZ	LYS	A	459	31.341	94.675	11.169	1.00	79.35
	945	N	ARG	A	460	26.406	96.194	15.001	1.00	52.32
	946	CA	ARG	A	460	25.035	95.951	15.377	1.00	47.59
	947	C	ARG	A	460	24.860	94.436	15.290	1.00	43.34
	948	O	ARG	A	460	25.477	93.761	14.462	1.00	40.40
	949	CB	ARG	A	460	24.104	96.726	14.456	1.00	49.27
	950	CG	ARG	A	460	24.275	98.216	14.671	1.00	56.23
	951	CD	ARG	A	460	23.659	99.006	13.532	1.00	63.20
	952	NE	ARG	A	460	23.997	100.426	13.596	1.00	68.02
	953	CZ	ARG	A	460	25.145	100.955	13.180	1.00	70.46
	954	NH1	ARG	A	460	26.094	100.185	12.656	1.00	72.23
	955	NH2	ARG	A	460	25.336	102.264	13.285	1.00	73.53
	956	N	THR	A	461	24.062	93.910	16.198	1.00	39.19
	957	CA	THR	A	461	23.879	92.474	16.278	1.00	36.81
	958	C	THR	A	461	22.447	92.004	16.401	1.00	34.03
	959	O	THR	A	461	21.631	92.607	17.110	1.00	33.96
	960	CB	THR	A	461	24.603	91.890	17.512	1.00	39.13
	961	OG1	THR	A	461	25.957	92.357	17.557	1.00	46.04
	962	CG2	THR	A	461	24.630	90.380	17.421	1.00	45.48
	963	N	LEU	A	462	22.157	90.904	15.714	1.00	29.84
	964	CA	LEU	A	462	20.853	90.267	15.788	1.00	28.03
	965	C	LEU	A	462	21.205	88.926	16.410	1.00	27.33
	966	O	LEU	A	462	22.307	88.414	16.207	1.00	24.47
	967	CB	LEU	A	462	20.223	90.074	14.403	1.00	25.97
	968	CG	LEU	A	462	19.888	91.362	13.635	1.00	33.39
	969	CD1	LEU	A	462	19.172	91.007	12.319	1.00	32.36
	970	CD2	LEU	A	462	19.014	92.263	14.483	1.00	30.72
	971	N	ALA	A	463	20.286	88.359	17.178	1.00	25.83
	972	CA	ALA	A	463	20.577	87.111	17.836	1.00	25.65
	973	C	ALA	A	463	19.330	86.279	17.957	1.00	26.32

	974	O	ALA	A	463	18.214	86.790	17.846	1.00	27.53
	975	CB	ALA	A	463	21.179	87.381	19.212	1.00	28.15
	976	N	CYS	A	464	19.518	84.992	18.195	1.00	21.23
45	977	CA	CYS	A	464	18.388	84.093	18.276	1.00	24.77
	978	C	CYS	A	464	18.599	83.016	19.314	1.00	22.14
	979	O	CYS	A	464	19.683	82.431	19.402	1.00	24.66
	980	CB	CYS	A	464	18.193	83.429	16.914	1.00	22.04
	981	SG	CYS	A	464	16.790	82.298	16.720	1.00	34.06
50	982	N	LEU	A	465	17.548	82.741	20.075	1.00	22.44
	983	CA	LEU	A	465	17.598	81.697	21.089	1.00	23.11
	984	C	LEU	A	465	16.644	80.615	20.641	1.00	22.43
	985	O	LEU	A	465	15.483	80.898	20.352	1.00	23.73
	986	CB	LEU	A	465	17.155	82.230	22.461	1.00	22.99
55	987	CG	LEU	A	465	16.810	81.177	23.538	1.00	19.04
	988	CD1	LEU	A	465	18.035	80.331	23.866	1.00	21.72
	989	CD2	LEU	A	465	16.347	81.884	24.818	1.00	28.23
	990	N	ILE	A	466	17.125	79.380	20.581	1.00	22.56
	991	CA	ILE	A	466	16.277	78.268	20.169	1.00	22.11
5	992	C	ILE	A	466	16.302	77.256	21.297	1.00	24.25
	993	O	ILE	A	466	17.375	76.815	21.706	1.00	24.93
	994	CB	ILE	A	466	16.781	77.654	18.861	1.00	22.15
	995	CG1	ILE	A	466	16.849	78.750	17.786	1.00	23.07
	996	CG2	ILE	A	466	15.822	76.525	18.416	1.00	25.24
10	997	CD1	ILE	A	466	17.509	78.318	16.496	1.00	33.12
	998	N	GLN	A	467	15.132	76.863	21.793	1.00	24.63
	999	CA	GLN	A	467	15.120	75.970	22.951	1.00	28.64
	1000	C	GLN	A	467	13.982	74.963	23.072	1.00	31.08
	1001	O	GLN	A	467	13.071	74.915	22.235	1.00	31.00
15	1002	CB	GLN	A	467	15.172	76.830	24.228	1.00	25.58
	1003	CG	GLN	A	467	13.943	77.727	24.404	1.00	25.53
	1004	CD	GLN	A	467	14.044	78.693	25.599	1.00	30.72
	1005	OE1	GLN	A	467	14.790	78.456	26.549	1.00	29.76
	1006	NE2	GLN	A	467	13.273	79.779	25.550	1.00	32.18
20	1007	N	ASN	A	468	14.083	74.147	24.123	1.00	33.71
	1008	CA	ASN	A	468	13.114	73.106	24.459	1.00	36.96
	1009	C	ASN	A	468	12.993	71.999	23.423	1.00	38.20
	1010	O	ASN	A	468	11.931	71.392	23.288	1.00	38.39
	1011	CB	ASN	A	468	11.731	73.719	24.676	1.00	41.06
25	1012	CG	ASN	A	468	11.748	74.837	25.686	1.00	46.41
	1013	OD1	ASN	A	468	12.372	74.721	26.741	1.00	50.82
	1014	ND2	ASN	A	468	11.052	75.928	25.376	1.00	53.31
	1015	N	PHE	A	469	14.065	71.732	22.685	1.00	35.74
	1016	CA	PHE	A	469	14.003	70.690	21.677	1.00	33.87
30	1017	C	PHE	A	469	14.804	69.453	22.056	1.00	33.63
	1018	O	PHE	A	469	15.727	69.513	22.860	1.00	34.78
	1019	CB	PHE	A	469	14.495	71.228	20.322	1.00	29.12
	1020	CG	PHE	A	469	15.926	71.691	20.324	1.00	26.27
	1021	CD1	PHE	A	469	16.959	70.792	20.133	1.00	22.45
35	1022	CD2	PHE	A	469	16.238	73.034	20.539	1.00	22.06
	1023	CE1	PHE	A	469	18.285	71.214	20.126	1.00	23.84
	1024	CE2	PHE	A	469	17.564	73.465	20.536	1.00	28.02
	1025	CZ	PHE	A	469	18.593	72.549	20.327	1.00	23.33
	1026	N	MET	A	470	14.431	68.327	21.466	1.00	35.64
40	1027	CA	MET	A	470	15.120	67.065	21.687	1.00	37.62
	1028	C	MET	A	470	14.684	66.104	20.596	1.00	36.36
	1029	O	MET	A	470	13.529	66.122	20.177	1.00	36.33
	1030	CB	MET	A	470	14.804	66.495	23.076	1.00	42.61
	1031	CG	MET	A	470	13.354	66.179	23.350	1.00	50.60
45	1032	SD	MET	A	470	13.141	65.744	25.113	1.00	66.08
	1033	CE	MET	A	470	13.780	64.056	25.134	1.00	66.35
	1034	N	PRO	A	471	15.613	65.283	20.079	1.00	34.63
	1035	CA	PRO	A	471	17.039	65.169	20.418	1.00	32.61

	1036	C	PRO	A	471	17.818	66.453	20.143	1.00	31.92
	1037	O	PRO	A	471	17.244	67.436	19.685	1.00	29.59
	1038	CB	PRO	A	471	17.520	64.015	19.538	1.00	33.95
	1039	CG	PRO	A	471	16.277	63.227	19.295	1.00	37.90
	1040	CD	PRO	A	471	15.246	64.291	19.058	1.00	34.78
	1041	N	GLU	A	472	19.128	66.413	20.386	1.00	32.28
	1042	CA	GLU	A	472	20.001	67.580	20.234	1.00	36.49
	1043	C	GLU	A	472	20.380	68.043	18.830	1.00	35.52
	1044	O	GLU	A	472	20.870	69.162	18.683	1.00	34.87
	1045	CB	GLU	A	472	21.302	67.377	21.015	1.00	41.97
	1046	CG	GLU	A	472	22.213	66.306	20.423	1.00	54.78
	1047	CD	GLU	A	472	23.527	66.144	21.184	1.00	62.41
	1048	OE1	GLU	A	472	23.603	66.579	22.356	1.00	67.26
	1049	OE2	GLU	A	472	24.481	65.566	20.613	1.00	64.96
	1050	N	ASP	A	473	20.161	67.221	17.805	1.00	34.38
	1051	CA	ASP	A	473	20.543	67.629	16.452	1.00	31.83
	1052	C	ASP	A	473	19.602	68.686	15.886	1.00	31.24
	1053	O	ASP	A	473	18.380	68.528	15.901	1.00	31.80
	1054	CB	ASP	A	473	20.621	66.420	15.516	1.00	34.73
	1055	CG	ASP	A	473	21.746	65.453	15.904	1.00	40.83
	1056	OD1	ASP	A	473	22.841	65.924	16.296	1.00	44.18
	1057	OD2	ASP	A	473	21.539	64.222	15.810	1.00	40.17
	1058	N	ILE	A	474	20.184	69.774	15.398	1.00	26.96
	1059	CA	ILE	A	474	19.393	70.856	14.854	1.00	25.39
	1060	C	ILE	A	474	20.225	71.715	13.892	1.00	24.74
	1061	O	ILE	A	474	21.436	71.824	14.031	1.00	25.20
	1062	CB	ILE	A	474	18.842	71.738	16.008	1.00	23.81
	1063	CG1	ILE	A	474	17.748	72.675	15.502	1.00	22.23
	1064	CG2	ILE	A	474	19.974	72.538	16.647	1.00	27.10
	1065	CD1	ILE	A	474	17.064	73.456	16.650	1.00	25.30
	1066	N	SER	A	475	19.570	72.288	12.891	1.00	23.27
	1067	CA	SER	A	475	20.252	73.170	11.952	1.00	22.17
	1068	C	SER	A	475	19.609	74.534	12.148	1.00	21.71
	1069	O	SER	A	475	18.393	74.649	12.224	1.00	20.84
	1070	CB	SER	A	475	20.049	72.721	10.507	1.00	20.43
	1071	OG	SER	A	475	20.589	71.436	10.294	1.00	30.00
	1072	N	VAL	A	476	20.442	75.558	12.213	1.00	21.76
	1073	CA	VAL	A	476	19.980	76.906	12.425	1.00	21.72
	1074	C	VAL	A	476	20.435	77.725	11.249	1.00	23.56
	1075	O	VAL	A	476	21.555	77.564	10.780	1.00	25.95
	1076	CB	VAL	A	476	20.606	77.513	13.715	1.00	21.56
	1077	CG1	VAL	A	476	20.157	78.975	13.878	1.00	18.70
	1078	CG2	VAL	A	476	20.197	76.685	14.934	1.00	20.99
	1079	N	GLN	A	477	19.574	78.606	10.764	1.00	25.16
	1080	CA	GLN	A	477	19.965	79.428	9.640	1.00	26.65
	1081	C	GLN	A	477	19.263	80.767	9.662	1.00	26.62
	1082	O	GLN	A	477	18.160	80.891	10.175	1.00	26.40
	1083	CB	GLN	A	477	19.701	78.683	8.325	1.00	31.51
	1084	CG	GLN	A	477	18.289	78.252	8.089	1.00	44.27
	1085	CD	GLN	A	477	18.188	77.095	7.084	1.00	47.76
	1086	OE1	GLN	A	477	17.104	76.786	6.598	1.00	50.57
	1087	NE2	GLN	A	477	19.317	76.449	6.787	1.00	47.32
	1088	N	TRP	A	478	19.941	81.780	9.146	1.00	27.41
	1089	CA	TRP	A	478	19.375	83.112	9.074	1.00	28.36
	1090	C	TRP	A	478	18.944	83.408	7.635	1.00	30.10
	1091	O	TRP	A	478	19.567	82.940	6.672	1.00	25.31
	1092	CB	TRP	A	478	20.404	84.139	9.533	1.00	28.76
	1093	CG	TRP	A	478	20.649	84.098	11.013	1.00	34.11
	1094	CD1	TRP	A	478	21.522	83.287	11.685	1.00	31.25
	1095	CD2	TRP	A	478	19.980	84.878	12.006	1.00	31.01
	1096	NE1	TRP	A	478	21.436	83.515	13.031	1.00	27.71
	1097	CE2	TRP	A	478	20.496	84.487	13.259	1.00	31.95

	1098	CE3	TRP	A	478	18.993	85.871	11.960	1.00	34.16
	1099	CZ2	TRP	A	478	20.055	85.058	14.463	1.00	25.26
	1100	CZ3	TRP	A	478	18.556	86.439	13.153	1.00	31.64
	1101	CH2	TRP	A	478	19.089	86.029	14.387	1.00	28.89
	1102	N	LEU	A	479	17.877	84.182	7.498	1.00	32.48
	1103	CA	LEU	A	479	17.355	84.551	6.187	1.00	37.36
	1104	C	LEU	A	479	16.943	86.016	6.140	1.00	40.42
	1105	O	LEU	A	479	16.448	86.560	7.123	1.00	40.14
	1106	CB	LEU	A	479	16.122	83.722	5.848	1.00	39.83
	1107	CG	LEU	A	479	16.044	82.254	6.258	1.00	44.57
	1108	CD1	LEU	A	479	14.713	81.710	5.810	1.00	52.98
	1109	CD2	LEU	A	479	17.161	81.470	5.634	1.00	50.71
	1110	N	HIS	A	480	17.152	86.653	4.998	1.00	43.05
	1111	CA	HIS	A	480	16.723	88.028	4.824	1.00	49.20
	1112	C	HIS	A	480	15.464	87.854	3.984	1.00	52.73
	1113	O	HIS	A	480	15.509	87.895	2.753	1.00	52.90
	1114	CB	HIS	A	480	17.756	88.846	4.057	1.00	52.25
	1115	CG	HIS	A	480	17.330	90.259	3.814	1.00	57.22
	1116	ND1	HIS	A	480	17.525	91.263	4.736	1.00	61.37
	1117	CD2	HIS	A	480	16.658	90.822	2.781	1.00	59.16
	1118	CE1	HIS	A	480	16.993	92.384	4.285	1.00	59.88
	1119	NE2	HIS	A	480	16.460	92.144	3.100	1.00	66.11
	1120	N	ASN	A	481	14.347	87.629	4.670	1.00	56.65
	1121	CA	ASN	A	481	13.057	87.394	4.030	1.00	59.93
	1122	C	ASN	A	481	13.009	85.940	3.581	1.00	59.65
	1123	O	ASN	A	481	13.031	85.029	4.405	1.00	61.04
	1124	CB	ASN	A	481	12.849	88.312	2.818	1.00	64.65
	1125	CG	ASN	A	481	12.578	89.748	3.210	1.00	72.38
	1126	OD1	ASN	A	481	11.636	90.037	3.953	1.00	74.96
	1127	ND2	ASN	A	481	13.401	90.662	2.707	1.00	75.60
	1128	N	GLU	A	482	12.975	85.728	2.273	1.00	58.97
	1129	CA	GLU	A	482	12.903	84.387	1.704	1.00	58.55
	1130	C	GLU	A	482	14.254	83.785	1.318	1.00	55.30
	1131	O	GLU	A	482	14.347	82.587	1.056	1.00	57.27
	1132	CB	GLU	A	482	11.993	84.424	0.473	1.00	65.42
	1133	CG	GLU	A	482	11.787	85.840	-0.072	1.00	73.94
	1134	CD	GLU	A	482	11.127	85.865	-1.432	1.00	80.29
	1135	OE1	GLU	A	482	11.770	85.432	-2.413	1.00	86.31
	1136	OE2	GLU	A	482	9.967	86.316	-1.520	1.00	82.73
	1137	N	VAL	A	483	15.299	84.603	1.286	1.00	50.25
	1138	CA	VAL	A	483	16.612	84.113	0.889	1.00	45.78
	1139	C	VAL	A	483	17.575	83.867	2.048	1.00	43.04
	1140	O	VAL	A	483	17.766	84.720	2.902	1.00	41.34
	1141	CB	VAL	A	483	17.261	85.073	-0.133	1.00	43.76
	1142	CG1	VAL	A	483	17.317	86.471	0.432	1.00	46.25
	1143	CG2	VAL	A	483	18.654	84.589	-0.494	1.00	41.37
	1144	N	GLN	A	484	18.188	82.688	2.050	1.00	42.30
	1145	CA	GLN	A	484	19.126	82.300	3.095	1.00	43.21
	1146	C	GLN	A	484	20.509	82.942	2.959	1.00	42.48
	1147	O	GLN	A	484	21.055	83.062	1.856	1.00	41.64
	1148	CB	GLN	A	484	19.269	80.774	3.129	1.00	45.96
	1149	CG	GLN	A	484	20.331	80.276	4.101	1.00	54.43
	1150	CD	GLN	A	484	20.427	78.760	4.159	1.00	59.02
	1151	OE1	GLN	A	484	21.400	78.209	4.677	1.00	59.71
	1152	NE2	GLN	A	484	19.410	78.078	3.636	1.00	61.46
	1153	N	LEU	A	485	21.061	83.361	4.094	1.00	38.99
	1154	CA	LEU	A	485	22.382	83.982	4.147	1.00	39.17
	1155	C	LEU	A	485	23.458	82.900	4.247	1.00	40.35

	1156	O	LEU	A	485	23.183	81.778	4.670	1.00	37.39
	1157	CB	LEU	A	485	22.493	84.895	5.375	1.00	37.16
	1158	CG	LEU	A	485	21.460	86.021	5.498	1.00	39.66
	1159	CD1	LEU	A	485	21.670	86.764	6.807	1.00	39.30
	1160	CD2	LEU	A	485	21.580	86.956	4.305	1.00	40.56
	1161	N	PRO	A	486	24.700	83.227	3.858	1.00	42.55
	1162	CA	PRO	A	486	25.772	82.234	3.942	1.00	46.30
	1163	C	PRO	A	486	25.940	81.850	5.412	1.00	49.32
	1164	O	PRO	A	486	25.748	82.684	6.294	1.00	48.81
	1165	CB	PRO	A	486	26.991	82.994	3.425	1.00	45.64
	1166	CG	PRO	A	486	26.413	84.068	2.572	1.00	45.29
	1167	CD	PRO	A	486	25.206	84.505	3.331	1.00	40.65
	1168	N	ASP	A	487	26.310	80.603	5.671	1.00	53.39
	1169	CA	ASP	A	487	26.507	80.135	7.038	1.00	57.75
	1170	C	ASP	A	487	27.603	80.940	7.750	1.00	57.25
	1171	O	ASP	A	487	27.424	81.395	8.887	1.00	57.75
	1172	CB	ASP	A	487	26.892	78.656	7.023	1.00	67.82
	1173	CG	ASP	A	487	26.821	78.023	8.397	1.00	76.17
	1174	OD1	ASP	A	487	27.291	78.655	9.366	1.00	84.77
	1175	OD2	ASP	A	487	26.303	76.889	8.508	1.00	86.94
	1176	N	ALA	A	488	28.727	81.122	7.065	1.00	54.64
	1177	CA	ALA	A	488	29.871	81.848	7.607	1.00	53.45
	1178	C	ALA	A	488	29.531	83.179	8.263	1.00	52.74
	1179	O	ALA	A	488	30.359	83.757	8.966	1.00	53.06
	1180	CB	ALA	A	488	30.892	82.070	6.515	1.00	53.75
	1181	N	ARG	A	489	28.313	83.662	8.044	1.00	50.96
	1182	CA	ARG	A	489	27.896	84.940	8.609	1.00	47.84
	1183	C	ARG	A	489	27.436	84.895	10.064	1.00	45.10
	1184	O	ARG	A	489	27.442	85.919	10.737	1.00	43.37
	1185	CB	ARG	A	489	26.792	85.554	7.746	1.00	48.99
	1186	CG	ARG	A	489	27.306	86.368	6.576	1.00	50.01
	1187	CD	ARG	A	489	27.173	87.839	6.873	1.00	50.36
	1188	NE	ARG	A	489	26.019	88.413	6.195	1.00	56.65
	1189	CZ	ARG	A	489	25.434	89.552	6.543	1.00	58.23
	1190	NH1	ARG	A	489	25.886	90.248	7.578	1.00	61.07
	1191	NH2	ARG	A	489	24.407	90.006	5.840	1.00	59.63
	1192	N	HIS	A	490	27.027	83.728	10.549	1.00	42.41
	1193	CA	HIS	A	490	26.576	83.635	11.934	1.00	41.63
	1194	C	HIS	A	490	27.390	82.648	12.766	1.00	39.71
	1195	O	HIS	A	490	28.129	81.832	12.235	1.00	41.30
	1196	CB	HIS	A	490	25.092	83.252	12.000	1.00	42.40
	1197	CG	HIS	A	490	24.793	81.880	11.486	1.00	43.27
	1198	ND1	HIS	A	490	24.423	81.634	10.181	1.00	42.27
	1199	CD2	HIS	A	490	24.821	80.674	12.101	1.00	44.41
	1200	CE1	HIS	A	490	24.236	80.338	10.014	1.00	39.88
	1201	NE2	HIS	A	490	24.470	79.732	11.166	1.00	45.37
	1202	N	SER	A	491	27.245	82.742	14.080	1.00	37.20
	1203	CA	SER	A	491	27.946	81.866	15.005	1.00	36.36
	1204	C	SER	A	491	26.915	81.199	15.927	1.00	33.06
	1205	O	SER	A	491	26.172	81.879	16.639	1.00	33.77
	1206	CB	SER	A	491	28.949	82.690	15.812	1.00	35.42
	1207	OG	SER	A	491	29.547	81.906	16.818	1.00	43.65
	1208	N	THR	A	492	26.878	79.872	15.912	1.00	29.90
	1209	CA	THR	A	492	25.927	79.105	16.717	1.00	29.91
	1210	C	THR	A	492	26.623	78.278	17.813	1.00	29.20
	1211	O	THR	A	492	27.609	77.604	17.548	1.00	30.85
	1212	CB	THR	A	492	25.094	78.153	15.802	1.00	29.85
	1213	OG1	THR	A	492	24.403	78.930	14.819	1.00	35.86
	1214	CG2	THR	A	492	24.059	77.366	16.602	1.00	28.05
	1215	N	THR	A	493	26.095	78.319	19.035	1.00	29.49
	1216	CA	THR	A	493	26.687	77.568	20.143	1.00	30.19
	1217	C	THR	A	493	26.305	76.099	20.044	1.00	32.39

	1218	O	THR	A	493	25.390	75.737	19.314	1.00	30.70
	1219	CB	THR	A	493	26.222	78.098	21.532	1.00	27.82
	1220	OG1	THR	A	493	24.794	78.008	21.640	1.00	30.48
	1221	CG2	THR	A	493	26.647	79.533	21.728	1.00	22.03
	1222	N	GLN	A	494	27.014	75.253	20.778	1.00	35.09
	1223	CA	GLN	A	494	26.721	73.821	20.770	1.00	38.19
	1224	C	GLN	A	494	25.509	73.568	21.651	1.00	36.48
	1225	O	GLN	A	494	25.330	74.240	22.668	1.00	35.75
	1226	CB	GLN	A	494	27.904	73.019	21.325	1.00	43.09
	1227	CG	GLN	A	494	29.167	73.098	20.490	1.00	58.35
	1228	CD	GLN	A	494	28.934	72.671	19.058	1.00	65.11
	1229	OE1	GLN	A	494	28.391	71.597	18.797	1.00	71.67
	1230	NE2	GLN	A	494	29.345	73.512	18.118	1.00	71.87
	1231	N	PRO	A	495	24.661	72.598	21.272	1.00	36.89
	1232	CA	PRO	A	495	23.470	72.278	22.063	1.00	38.37
	1233	C	PRO	A	495	23.863	71.991	23.513	1.00	40.80
	1234	O	PRO	A	495	24.837	71.286	23.773	1.00	40.76
	1235	CB	PRO	A	495	22.920	71.043	21.371	1.00	37.83
	1236	CG	PRO	A	495	23.300	71.285	19.926	1.00	40.41
	1237	CD	PRO	A	495	24.716	71.791	20.039	1.00	35.81
	1238	N	ARG	A	496	23.120	72.560	24.450	1.00	42.05
	1239	CA	ARG	A	496	23.392	72.345	25.860	1.00	47.69
	1240	C	ARG	A	496	22.146	71.828	26.558	1.00	51.66
	1241	O	ARG	A	496	21.042	72.317	26.316	1.00	51.95
	1242	CB	ARG	A	496	23.849	73.646	26.516	1.00	45.81
	1243	CG	ARG	A	496	25.283	74.001	26.208	1.00	51.53
	1244	CD	ARG	A	496	25.653	75.383	26.709	1.00	53.72
	1245	NE	ARG	A	496	27.046	75.425	27.137	1.00	57.50
	1246	CZ	ARG	A	496	27.478	74.992	28.317	1.00	58.59
	1247	NH1	ARG	A	496	26.626	74.489	29.199	1.00	57.22
	1248	NH2	ARG	A	496	28.768	75.058	28.612	1.00	65.31
	1249	N	LYS	A	497	22.319	70.827	27.413	1.00	56.98
	1250	CA	LYS	A	497	21.192	70.265	28.147	1.00	61.91
	1251	C	LYS	A	497	20.733	71.299	29.145	1.00	63.97
	1252	O	LYS	A	497	21.405	72.300	29.371	1.00	64.61
	1253	CB	LYS	A	497	21.597	69.013	28.928	1.00	66.35
	1254	CG	LYS	A	497	21.819	67.752	28.113	1.00	74.14
	1255	CD	LYS	A	497	22.241	66.607	29.034	1.00	80.69
	1256	CE	LYS	A	497	22.408	65.296	28.286	1.00	84.48
	1257	NZ	LYS	A	497	22.861	64.215	29.211	1.00	88.26
	1258	N	THR	A	498	19.583	71.045	29.748	1.00	67.67
	1259	CA	THR	A	498	19.028	71.931	30.758	1.00	71.26
	1260	C	THR	A	498	18.316	71.050	31.760	1.00	73.04
	1261	O	THR	A	498	18.610	69.857	31.864	1.00	72.83
	1262	CB	THR	A	498	18.015	72.921	30.155	1.00	71.80
	1263	OG1	THR	A	498	17.045	72.208	29.379	1.00	71.58
	1264	CG2	THR	A	498	18.722	73.930	29.281	1.00	73.61
	1265	N	LYS	A	499	17.380	71.638	32.495	1.00	75.57
	1266	CA	LYS	A	499	16.607	70.895	33.480	1.00	77.62
	1267	C	LYS	A	499	15.458	70.173	32.779	1.00	77.92
	1268	O	LYS	A	499	14.504	70.809	32.332	1.00	79.19
	1269	CB	LYS	A	499	16.042	71.848	34.533	1.00	80.22
	1270	CG	LYS	A	499	17.069	72.428	35.496	1.00	81.04
	1271	CD	LYS	A	499	17.507	71.397	36.529	1.00	83.26
	1272	CE	LYS	A	499	18.368	72.031	37.613	1.00	84.81
	1273	NZ	LYS	A	499	18.736	71.055	38.675	1.00	86.04
	1274	N	GLY	A	500	15.566	68.852	32.667	1.00	76.91
	1275	CA	GLY	A	500	14.523	68.056	32.039	1.00	75.83
	1276	C	GLY	A	500	14.040	68.459	30.655	1.00	75.14
	1277	O	GLY	A	500	14.024	67.629	29.745	1.00	75.52
	1278	N	SER	A	501	13.642	69.718	30.495	1.00	73.08
	1279	CA	SER	A	501	13.132	70.230	29.225	1.00	71.65

	1280	C	SER	A	501	13.764	69.592	27.994	1.00	68.64
	1281	O	SER	A	501	13.085	68.910	27.223	1.00	71.13
	1282	CB	SER	A	501	13.321	71.746	29.147	1.00	74.43
	1283	OG	SER	A	501	14.667	72.076	28.859	1.00	80.92
	1284	N	GLY	A	502	15.060	69.814	27.810	1.00	63.14
	1285	CA	GLY	A	502	15.741	69.256	26.657	1.00	54.62
	1286	C	GLY	A	502	16.982	70.048	26.297	1.00	48.04
	1287	O	GLY	A	502	17.917	70.131	27.094	1.00	48.08
	1288	N	PHE	A	503	17.001	70.642	25.106	1.00	40.50
	1289	CA	PHE	A	503	18.173	71.411	24.692	1.00	33.81
	1290	C	PHE	A	503	17.908	72.827	24.212	1.00	28.39
	1291	O	PHE	A	503	16.789	73.192	23.856	1.00	26.35
	1292	CB	PHE	A	503	18.938	70.681	23.583	1.00	35.09
	1293	CG	PHE	A	503	19.452	69.337	23.981	1.00	34.16
	1294	CD1	PHE	A	503	18.630	68.219	23.926	1.00	35.05
	1295	CD2	PHE	A	503	20.755	69.189	24.430	1.00	35.90
	1296	CE1	PHE	A	503	19.099	66.967	24.317	1.00	36.00
	1297	CE2	PHE	A	503	21.238	67.944	24.826	1.00	40.04
	1298	CZ	PHE	A	503	20.408	66.829	24.771	1.00	38.82
	1299	N	PHE	A	504	18.967	73.625	24.216	1.00	26.16
	1300	CA	PHE	A	504	18.891	74.988	23.731	1.00	25.00
	1301	C	PHE	A	504	20.182	75.314	23.004	1.00	26.57
	1302	O	PHE	A	504	21.221	74.708	23.267	1.00	26.73
	1303	CB	PHE	A	504	18.640	75.984	24.858	1.00	22.46
	1304	CG	PHE	A	504	19.834	76.270	25.718	1.00	27.70
	1305	CD1	PHE	A	504	20.674	77.340	25.433	1.00	28.94
	1306	CD2	PHE	A	504	20.083	75.514	26.857	1.00	31.34
	1307	CE1	PHE	A	504	21.743	77.662	26.273	1.00	30.08
	1308	CE2	PHE	A	504	21.151	75.828	27.704	1.00	32.65
	1309	CZ	PHE	A	504	21.979	76.909	27.403	1.00	32.80
	1310	N	VAL	A	505	20.091	76.270	22.085	1.00	23.68
	1311	CA	VAL	A	505	21.211	76.705	21.286	1.00	24.67
	1312	C	VAL	A	505	21.041	78.215	21.072	1.00	23.86
	1313	O	VAL	A	505	19.928	78.725	21.049	1.00	21.24
	1314	CB	VAL	A	505	21.208	75.926	19.939	1.00	27.95
	1315	CG1	VAL	A	505	20.134	76.464	19.020	1.00	25.61
	1316	CG2	VAL	A	505	22.558	75.957	19.314	1.00	33.51
	1317	N	PHE	A	506	22.146	78.936	20.959	1.00	26.20
	1318	CA	PHE	A	506	22.086	80.382	20.754	1.00	26.10
	1319	C	PHE	A	506	22.846	80.745	19.479	1.00	24.83
	1320	O	PHE	A	506	23.928	80.231	19.241	1.00	25.52
	1321	CB	PHE	A	506	22.725	81.104	21.939	1.00	28.18
	1322	CG	PHE	A	506	22.758	82.593	21.797	1.00	35.33
	1323	CD1	PHE	A	506	21.620	83.355	22.020	1.00	42.56
	1324	CD2	PHE	A	506	23.937	83.241	21.443	1.00	40.04
	1325	CE1	PHE	A	506	21.660	84.746	21.892	1.00	44.70
	1326	CE2	PHE	A	506	23.987	84.623	21.311	1.00	40.54
	1327	CZ	PHE	A	506	22.851	85.377	21.536	1.00	42.12
	1328	N	SER	A	507	22.290	81.639	18.673	1.00	24.69
	1329	CA	SER	A	507	22.941	82.050	17.426	1.00	24.73
	1330	C	SER	A	507	23.065	83.578	17.355	1.00	26.40
	1331	O	SER	A	507	22.113	84.292	17.609	1.00	25.99
	1332	CB	SER	A	507	22.151	81.521	16.221	1.00	22.19
	1333	OG	SER	A	507	22.740	81.947	15.009	1.00	30.30
	1334	N	ARG	A	508	24.255	84.062	17.009	1.00	26.98
	1335	CA	ARG	A	508	24.545	85.496	16.913	1.00	25.95
	1336	C	ARG	A	508	24.851	85.911	15.463	1.00	24.97
	1337	O	ARG	A	508	25.621	85.250	14.785	1.00	24.35
	1338	CB	ARG	A	508	25.755	85.801	17.790	1.00	21.97
	1339	CG	ARG	A	508	26.249	87.235	17.756	1.00	25.32
	1340	CD	ARG	A	508	27.474	87.372	18.656	1.00	25.67
	1341	NE	ARG	A	508	27.898	88.758	18.788	1.00	36.00

	1342	CZ	ARG	A	508	28.757	89.357	17.972	1.00	36.06
	1343	NH1	ARG	A	508	29.293	88.682	16.963	1.00	34.19
	1344	NH2	ARG	A	508	29.062	90.633	18.157	1.00	34.70
	1345	N	LEU	A	509	24.269	87.017	15.001	1.00	26.44
	1346	CA	LEU	A	509	24.492	87.479	13.621	1.00	28.45
	1347	C	LEU	A	509	24.794	88.973	13.540	1.00	28.87
	1348	O	LEU	A	509	23.893	89.797	13.699	1.00	30.99
	1349	CB	LEU	A	509	23.259	87.177	12.758	1.00	27.28
	1350	CG	LEU	A	509	23.270	87.733	11.321	1.00	31.90
	1351	CD1	LEU	A	509	24.284	86.985	10.453	1.00	29.48
	1352	CD2	LEU	A	509	21.886	87.599	10.732	1.00	28.89
	1353	N	GLU	A	510	26.054	89.323	13.288	1.00	31.92
	1354	CA	GLU	A	510	26.448	90.728	13.189	1.00	34.67
	1355	C	GLU	A	510	26.005	91.290	11.845	1.00	36.35
	1356	O	GLU	A	510	26.199	90.652	10.812	1.00	34.66
	1357	CB	GLU	A	510	27.970	90.875	13.343	1.00	41.07
	1358	CG	GLU	A	510	28.510	90.383	14.696	1.00	54.35
	1359	CD	GLU	A	510	29.997	90.675	14.911	1.00	58.86
	1360	OE1	GLU	A	510	30.811	90.364	14.013	1.00	61.22
	1361	OE2	GLU	A	510	30.349	91.207	15.989	1.00	61.34
	1362	N	VAL	A	511	25.406	92.479	11.852	1.00	36.50
	1363	CA	VAL	A	511	24.935	93.069	10.606	1.00	38.05
	1364	C	VAL	A	511	25.370	94.516	10.408	1.00	42.41
	1365	O	VAL	A	511	25.744	95.205	11.368	1.00	41.92
	1366	CB	VAL	A	511	23.403	93.012	10.508	1.00	31.84
	1367	CG1	VAL	A	511	22.927	91.585	10.669	1.00	32.42
	1368	CG2	VAL	A	511	22.787	93.913	11.553	1.00	26.87
	1369	N	THR	A	512	25.310	94.967	9.154	1.00	43.58
	1370	CA	THR	A	512	25.697	96.331	8.808	1.00	48.37
	1371	C	THR	A	512	24.602	97.306	9.201	1.00	50.53
	1372	O	THR	A	512	23.487	96.894	9.516	1.00	51.77
	1373	CB	THR	A	512	25.956	96.475	7.303	1.00	48.57
	1374	OG1	THR	A	512	24.766	96.140	6.581	1.00	46.96
	1375	CG2	THR	A	512	27.085	95.554	6.866	1.00	45.82
	1376	N	ARG	A	513	24.922	98.598	9.188	1.00	53.29
	1377	CA	ARG	A	513	23.952	99.629	9.544	1.00	55.54
	1378	C	ARG	A	513	22.781	99.557	8.577	1.00	55.38
	1379	O	ARG	A	513	21.623	99.741	8.962	1.00	55.22
	1380	CB	ARG	A	513	24.594	101.018	9.464	1.00	59.23
	1381	CG	ARG	A	513	23.999	102.037	10.428	1.00	65.98
	1382	CD	ARG	A	513	22.519	102.274	10.184	1.00	74.12
	1383	NE	ARG	A	513	21.858	102.827	11.365	1.00	80.97
	1384	CZ	ARG	A	513	20.581	103.197	11.413	1.00	83.64
	1385	NH1	ARG	A	513	19.809	103.084	10.340	1.00	86.02
	1386	NH2	ARG	A	513	20.072	103.673	12.543	1.00	85.44
	1387	N	ALA	A	514	23.099	99.285	7.317	1.00	55.03
	1388	CA	ALA	A	514	22.096	99.186	6.268	1.00	55.46
	1389	C	ALA	A	514	21.061	98.104	6.571	1.00	56.10
	1390	O	ALA	A	514	19.866	98.390	6.674	1.00	56.61
	1391	CB	ALA	A	514	22.775	98.908	4.927	1.00	54.05
	1392	N	GLU	A	515	21.509	96.859	6.712	1.00	55.46
	1393	CA	GLU	A	515	20.575	95.781	6.995	1.00	55.34
	1394	C	GLU	A	515	19.949	95.951	8.371	1.00	54.83
	1395	O	GLU	A	515	18.877	95.410	8.644	1.00	52.33
	1396	CB	GLU	A	515	21.265	94.413	6.868	1.00	57.76
	1397	CG	GLU	A	515	22.716	94.379	7.312	1.00	62.58
	1398	CD	GLU	A	515	23.416	93.082	6.937	1.00	63.27
	1399	OE1	GLU	A	515	23.168	92.565	5.829	1.00	64.89
	1400	OE2	GLU	A	515	24.228	92.586	7.741	1.00	66.59
	1401	N	TRP	A	516	20.608	96.716	9.234	1.00	55.79
	1402	CA	TRP	A	516	20.072	96.956	10.566	1.00	57.81
	1403	C	TRP	A	516	18.818	97.822	10.464	1.00	58.51

	1404	C	TRP	A	516	17.988	97.822	11.374	1.00	57.71
	1405	CB	TRP	A	516	21.101	97.649	11.466	1.00	61.48
	1406	CG	TRP	A	516	20.738	97.544	12.913	1.00	66.54
	1407	CD1	TRP	A	516	20.823	96.428	13.697	1.00	67.26
	1408	CD2	TRP	A	516	20.140	98.561	13.725	1.00	69.56
	1409	NE1	TRP	A	516	20.309	96.685	14.946	1.00	71.76
	1410	CE2	TRP	A	516	19.882	97.987	14.990	1.00	70.88
	1411	CE3	TRP	A	516	19.793	99.900	13.507	1.00	70.94
	1412	CZ2	TRP	A	516	19.292	98.706	16.034	1.00	73.50
	1413	CZ3	TRP	A	516	19.204	100.618	14.548	1.00	74.37
	1414	CH2	TRP	A	516	18.961	100.016	15.796	1.00	74.71
	1415	N	GLU	A	517	18.682	98.553	9.356	1.00	59.66
	1416	CA	GLU	A	517	17.515	99.409	9.128	1.00	61.72
	1417	C	GLU	A	517	16.301	98.565	8.746	1.00	59.87
	1418	O	GLU	A	517	15.159	98.994	8.904	1.00	58.60
	1419	CB	GLU	A	517	17.782	100.418	8.003	1.00	68.82
	1420	CG	GLU	A	517	18.988	101.316	8.221	1.00	80.60
	1421	CD	GLU	A	517	19.148	102.358	7.124	1.00	87.42
	1422	OE1	GLU	A	517	18.472	102.231	6.079	1.00	94.80
	1423	OE2	GLU	A	517	19.955	103.299	7.300	1.00	95.35
	1424	N	GLN	A	518	16.555	97.366	8.233	1.00	57.92
	1425	CA	GLN	A	518	15.480	96.468	7.836	1.00	55.74
	1426	C	GLN	A	518	15.543	95.184	8.664	1.00	54.32
	1427	O	GLN	A	518	15.207	94.102	8.176	1.00	52.85
	1428	CB	GLN	A	518	15.600	96.146	6.355	1.00	54.10
	1429	N	LYS	A	519	15.954	95.313	9.924	1.00	52.69
	1430	CA	LYS	A	519	16.082	94.152	10.791	1.00	52.35
	1431	C	LYS	A	519	14.781	93.394	10.941	1.00	51.69
	1432	O	LYS	A	519	14.778	92.203	11.246	1.00	49.61
	1433	CB	LYS	A	519	16.617	94.561	12.163	1.00	54.31
	1434	CG	LYS	A	519	15.688	95.395	13.012	1.00	55.80
	1435	CD	LYS	A	519	16.438	95.877	14.241	1.00	60.32
	1436	CE	LYS	A	519	15.598	96.806	15.089	1.00	64.05
	1437	NZ	LYS	A	519	16.409	97.377	16.202	1.00	70.92
	1438	N	ASP	A	520	13.676	94.089	10.712	1.00	52.66
	1439	CA	ASP	A	520	12.349	93.495	10.812	1.00	54.22
	1440	C	ASP	A	520	12.204	92.391	9.764	1.00	53.07
	1441	O	ASP	A	520	11.336	91.525	9.871	1.00	52.75
	1442	CB	ASP	A	520	11.289	94.568	10.563	1.00	61.14
	1443	CG	ASP	A	520	11.821	95.980	10.792	1.00	71.19
	1444	OD1	ASP	A	520	12.193	96.300	11.945	1.00	76.53
	1445	OD2	ASP	A	520	11.871	96.766	9.817	1.00	72.86
	1446	N	GLU	A	521	13.067	92.423	8.757	1.00	51.01
	1447	CA	GLU	A	521	13.018	91.443	7.684	1.00	50.49
	1448	C	GLU	A	521	13.886	90.206	7.899	1.00	47.73
	1449	O	GLU	A	521	13.762	89.228	7.165	1.00	48.58
	1450	CB	GLU	A	521	13.400	92.107	6.362	1.00	52.54
	1451	CG	GLU	A	521	12.423	93.173	5.901	1.00	60.11
	1452	CD	GLU	A	521	12.901	93.895	4.658	1.00	65.41
	1453	OE1	GLU	A	521	13.103	93.239	3.614	1.00	67.98
	1454	OE2	GLU	A	521	13.079	95.129	4.726	1.00	73.58
	1455	N	PHE	A	522	14.772	90.241	8.887	1.00	42.66
	1456	CA	PHE	A	522	15.615	89.081	9.137	1.00	38.90
	1457	C	PHE	A	522	14.847	88.017	9.892	1.00	35.93
	1458	O	PHE	A	522	14.021	88.324	10.755	1.00	38.85
	1459	CB	PHE	A	522	16.884	89.478	9.886	1.00	36.56
	1460	CG	PHE	A	522	17.890	90.181	9.019	1.00	39.04
	1461	CD1	PHE	A	522	17.673	91.494	8.605	1.00	42.28
	1462	CD2	PHE	A	522	19.026	89.513	8.561	1.00	36.78
	1463	CE1	PHE	A	522	18.571	92.132	7.738	1.00	44.30
	1464	CE2	PHE	A	522	19.927	90.139	7.695	1.00	40.92
	1465	CZ	PHE	A	522	19.699	91.454	7.283	1.00	39.51

	1466	N	ILE	A	523	15.108	86.763	9.545	1.00	31.27
	1467	CA	ILE	A	523	14.427	85.641	10.156	1.00	29.65
	1468	C	ILE	A	523	15.389	84.551	10.617	1.00	29.13
	1469	O	ILE	A	523	16.364	84.240	9.936	1.00	27.36
	1470	CB	ILE	A	523	13.420	85.033	9.163	1.00	34.21
	1471	CG1	ILE	A	523	12.349	86.072	8.818	1.00	37.38
	1472	CG2	ILE	A	523	12.804	83.773	9.736	1.00	34.94
	1473	CD1	ILE	A	523	11.373	85.619	7.746	1.00	38.56
	1474	N	CYS	A	524	15.102	83.990	11.789	1.00	26.34
	1475	CA	CYS	A	524	15.901	82.914	12.361	1.00	27.10
	1476	C	CYS	A	524	15.100	81.654	12.138	1.00	26.67
	1477	O	CYS	A	524	13.945	81.590	12.531	1.00	27.58
	1478	CB	CYS	A	524	16.103	83.127	13.874	1.00	24.27
	1479	SG	CYS	A	524	16.974	81.777	14.737	1.00	37.60
	1480	N	ARG	A	525	15.714	80.649	11.528	1.00	26.37
	1481	CA	ARG	A	525	15.024	79.406	11.244	1.00	26.35
	1482	C	ARG	A	525	15.713	78.181	11.796	1.00	26.72
	1483	O	ARG	A	525	16.929	78.039	11.700	1.00	29.04
	1484	CB	ARG	A	525	14.852	79.224	9.739	1.00	29.81
	1485	CG	ARG	A	525	14.207	77.887	9.372	1.00	35.40
	1486	CD	ARG	A	525	13.542	77.948	8.001	1.00	46.51
	1487	NE	ARG	A	525	14.487	77.804	6.907	1.00	50.77
	1488	CZ	ARG	A	525	14.221	78.139	5.649	1.00	55.09
	1489	NH1	ARG	A	525	13.035	78.649	5.337	1.00	54.58
	1490	NH2	ARG	A	525	15.136	77.950	4.703	1.00	56.77
	1491	N	ALA	A	526	14.920	77.289	12.369	1.00	25.38
	1492	CA	ALA	A	526	15.458	76.072	12.920	1.00	25.38
	1493	C	ALA	A	526	14.872	74.879	12.175	1.00	25.99
	1494	O	ALA	A	526	13.667	74.849	11.890	1.00	25.50
	1495	CB	ALA	A	526	15.116	75.971	14.404	1.00	25.98
	1496	N	VAL	A	527	15.728	73.916	11.841	1.00	23.84
	1497	CA	VAL	A	527	15.267	72.705	11.198	1.00	25.15
	1498	C	VAL	A	527	15.522	71.628	12.220	1.00	26.30
	1499	O	VAL	A	527	16.642	71.481	12.706	1.00	26.20
	1500	CB	VAL	A	527	16.043	72.365	9.923	1.00	24.43
	1501	CG1	VAL	A	527	15.610	71.012	9.439	1.00	26.95
	1502	CG2	VAL	A	527	15.781	73.409	8.849	1.00	28.13
	1503	N	HIS	A	528	14.485	70.862	12.531	1.00	26.24
	1504	CA	HIS	A	528	14.582	69.828	13.536	1.00	29.14
	1505	C	HIS	A	528	13.498	68.778	13.295	1.00	31.86
	1506	O	HIS	A	528	12.384	69.091	12.861	1.00	31.05
	1507	CB	HIS	A	528	14.428	70.479	14.921	1.00	29.03
	1508	CG	HIS	A	528	14.518	69.523	16.065	1.00	29.34
	1509	ND1	HIS	A	528	13.491	68.666	16.404	1.00	33.33
	1510	CD2	HIS	A	528	15.510	69.283	16.956	1.00	28.93
	1511	CE1	HIS	A	528	13.845	67.945	17.449	1.00	26.07
	1512	NE2	HIS	A	528	15.070	68.298	17.805	1.00	32.19
	1513	N	GLU	A	529	13.843	67.536	13.599	1.00	34.08
	1514	CA	GLU	A	529	12.964	66.393	13.424	1.00	39.76
	1515	C	GLU	A	529	11.563	66.490	14.034	1.00	41.50
	1516	O	GLU	A	529	10.580	66.190	13.360	1.00	41.48
	1517	CB	GLU	A	529	13.641	65.138	13.978	1.00	43.03
	1518	CG	GLU	A	529	12.702	63.935	14.014	1.00	56.19
	1519	CD	GLU	A	529	13.239	62.773	14.826	1.00	62.66
	1520	OE1	GLU	A	529	12.489	61.788	15.007	1.00	63.52
	1521	OE2	GLU	A	529	14.402	62.842	15.281	1.00	65.43
	1522	N	ALA	A	530	11.479	66.897	15.300	1.00	42.51
	1523	CA	ALA	A	530	10.201	66.978	16.006	1.00	46.03
	1524	C	ALA	A	530	9.269	68.105	15.596	1.00	49.29
	1525	O	ALA	A	530	8.124	68.153	16.044	1.00	50.87
	1526	CB	ALA	A	530	10.443	67.043	17.513	1.00	39.71
	1527	N	ALA	A	531	9.751	69.005	14.748	1.00	52.89

	1528	CA	ALA	A	531	8.949	70.133	14.302	1.00	56.14
	1529	C	ALA	A	531	8.030	69.799	13.124	1.00	59.66
	1530	O	ALA	A	531	8.258	70.243	12.004	1.00	61.00
	1531	CB	ALA	A	531	9.864	71.295	13.938	1.00	52.83
	1532	N	SER	A	532	6.992	69.012	13.370	1.00	63.07
	1533	CA	SER	A	532	6.056	68.673	12.305	1.00	66.03
	1534	C	SER	A	532	5.006	69.778	12.250	1.00	66.08
	1535	O	SER	A	532	4.569	70.283	13.286	1.00	65.35
	1536	CB	SER	A	532	5.384	67.330	12.593	1.00	68.98
	1537	OG	SER	A	532	4.526	67.416	13.716	1.00	74.64
	1538	N	PRO	A	533	4.581	70.173	11.043	1.00	66.51
	1539	CA	PRO	A	533	4.931	69.713	9.696	1.00	65.99
	1540	C	PRO	A	533	6.251	70.226	9.117	1.00	63.48
	1541	O	PRO	A	533	6.760	71.273	9.518	1.00	64.33
	1542	CB	PRO	A	533	3.757	70.203	8.873	1.00	69.06
	1543	CG	PRO	A	533	3.539	71.556	9.471	1.00	71.08
	1544	CD	PRO	A	533	3.570	71.242	10.963	1.00	70.23
	1545	N	SER	A	534	6.783	69.466	8.165	1.00	59.21
	1546	CA	SER	A	534	8.009	69.804	7.452	1.00	55.01
	1547	C	SER	A	534	9.274	70.148	8.248	1.00	50.27
	1548	O	SER	A	534	10.130	70.875	7.753	1.00	48.58
	1549	CB	SER	A	534	7.706	70.934	6.475	1.00	58.20
	1550	OG	SER	A	534	7.074	72.013	7.138	1.00	63.36
	1551	N	GLN	A	535	9.387	69.616	9.461	1.00	44.89
	1552	CA	GLN	A	535	10.543	69.829	10.330	1.00	42.88
	1553	C	GLN	A	535	11.194	71.205	10.277	1.00	41.55
	1554	O	GLN	A	535	12.419	71.321	10.294	1.00	40.80
	1555	CB	GLN	A	535	11.633	68.769	10.080	1.00	37.08
	1556	CG	GLN	A	535	11.302	67.731	9.056	1.00	47.40
	1557	CD	GLN	A	535	10.101	66.916	9.431	1.00	44.36
	1558	OE1	GLN	A	535	9.193	66.738	8.625	1.00	47.59
	1559	NE2	GLN	A	535	10.079	66.415	10.664	1.00	54.70
	1560	N	THR	A	536	10.387	72.252	10.226	1.00	39.97
	1561	CA	THR	A	536	10.950	73.588	10.207	1.00	40.62
	1562	C	THR	A	536	10.113	74.575	11.023	1.00	37.57
	1563	O	THR	A	536	8.893	74.558	10.975	1.00	40.85
	1564	CB	THR	A	536	11.137	74.092	8.747	1.00	42.38
	1565	OG1	THR	A	536	11.458	75.488	8.763	1.00	44.59
	1566	CG2	THR	A	536	9.881	73.870	7.932	1.00	49.65
	1567	N	VAL	A	537	10.788	75.410	11.801	1.00	35.29
	1568	CA	VAL	A	537	10.147	76.418	12.632	1.00	31.25
	1569	C	VAL	A	537	10.996	77.678	12.537	1.00	29.01
	1570	O	VAL	A	537	12.218	77.615	12.699	1.00	30.11
	1571	CB	VAL	A	537	10.106	75.996	14.117	1.00	34.80
	1572	CG1	VAL	A	537	9.452	77.084	14.939	1.00	35.52
	1573	CG2	VAL	A	537	9.341	74.712	14.278	1.00	37.19
	1574	N	GLN	A	538	10.365	78.820	12.292	1.00	26.73
	1575	CA	GLN	A	538	11.107	80.067	12.167	1.00	26.74
	1576	C	GLN	A	538	10.376	81.271	12.732	1.00	27.53
	1577	O	GLN	A	538	9.169	81.249	12.902	1.00	29.89
	1578	CB	GLN	A	538	11.424	80.335	10.700	1.00	28.48
	1579	CG	GLN	A	538	10.208	80.624	9.834	1.00	25.88
	1580	CD	GLN	A	538	10.595	80.853	8.378	1.00	28.51
	1581	OE1	GLN	A	538	11.390	80.102	7.810	1.00	31.66
	1582	NE2	GLN	A	538	10.035	81.885	7.772	1.00	27.39
	1583	N	ARG	A	539	11.113	82.334	13.013	1.00	28.05
	1584	CA	ARG	A	539	10.493	83.530	13.535	1.00	30.72
	1585	C	ARG	A	539	11.288	84.742	13.114	1.00	31.33
	1586	O	ARG	A	539	12.517	84.703	13.077	1.00	32.42
	1587	CB	ARG	A	539	10.420	83.463	15.061	1.00	36.30
	1588	CG	ARG	A	539	9.488	84.476	15.686	1.00	45.60
	1589	CD	ARG	A	539	8.741	83.829	16.830	1.00	57.97

	1590	NE	ARG	A	539	8.118	82.591	16.371	1.00	69.46
	1591	CZ	ARG	A	539	7.453	81.745	17.150	1.00	78.18
55	1592	NH1	ARG	A	539	7.316	81.996	18.447	1.00	83.01
	1593	NH2	ARG	A	539	6.927	80.641	16.630	1.00	81.89
	1594	N	ALA	A	540	10.578	85.818	12.799	1.00	31.92
	1595	CA	ALA	A	540	11.207	87.054	12.383	1.00	34.50
	1596	C	ALA	A	540	11.691	87.774	13.634	1.00	36.68
5	1597	O	ALA	A	540	11.190	87.532	14.739	1.00	34.62
	1598	CB	ALA	A	540	10.209	87.907	11.621	1.00	33.91
	1599	N	VAL	A	541	12.694	88.626	13.460	1.00	39.73
	1600	CA	VAL	A	541	13.254	89.386	14.572	1.00	44.47
	1601	C	VAL	A	541	12.164	90.249	15.218	1.00	46.91
10	1602	O	VAL	A	541	11.595	91.124	14.573	1.00	44.53
	1603	CB	VAL	A	541	14.415	90.295	14.090	1.00	42.49
	1604	CG1	VAL	A	541	14.715	91.358	15.130	1.00	47.96
	1605	CG2	VAL	A	541	15.655	89.460	13.831	1.00	42.43
	1606	N	SER	A	542	11.869	89.997	16.489	1.00	52.25
15	1607	CA	SER	A	542	10.840	90.771	17.174	1.00	60.05
	1608	C	SER	A	542	11.374	92.174	17.421	1.00	64.25
	1609	O	SER	A	542	12.550	92.353	17.743	1.00	65.22
	1610	CB	SER	A	542	10.443	90.110	18.500	1.00	60.43
	1611	OG	SER	A	542	11.530	90.076	19.404	1.00	65.30
20	1612	N	VAL	A	543	10.510	93.168	17.256	1.00	68.19
	1613	CA	VAL	A	543	10.906	94.557	17.444	1.00	72.45
	1614	C	VAL	A	543	9.828	95.323	18.202	1.00	74.32
	1615	O	VAL	A	543	8.970	95.979	17.603	1.00	75.99
	1616	CB	VAL	A	543	11.148	95.247	16.084	1.00	74.41
25	1617	CG1	VAL	A	543	11.530	96.705	16.299	1.00	76.37
	1618	CG2	VAL	A	543	12.233	94.514	15.318	1.00	75.78
	1619	O	HOH	A	1	24.509	77.358	12.191	1.00	54.75
	1620	O	HOH	A	2	7.537	85.444	12.546	1.00	37.27
	1621	O	HOH	A	3	26.419	96.436	20.705	1.00	46.90
30	1622	O	HOH	A	4	27.452	65.238	9.563	1.00	44.93
	1623	O	HOH	A	5	8.585	79.087	17.993	1.00	46.77
	1624	O	HOH	A	6	22.224	80.929	7.089	1.00	40.32
	1625	O	HOH	A	7	17.272	54.803	2.090	1.00	50.21
	1626	O	HOH	A	8	30.340	75.004	30.685	1.00	61.75
35	1627	O	HOH	A	9	24.537	65.977	6.710	1.00	39.17
	1628	O	HOH	A	10	16.841	94.781	2.897	1.00	64.36
	1629	O	HOH	A	11	22.950	61.704	0.621	1.00	45.74
	1630	O	HOH	A	12	28.469	65.195	7.094	1.00	39.34
	1631	O	HOH	A	13	53.771	76.970	5.717	1.00	56.15
40	1632	O	HOH	A	14	28.128	87.403	13.055	1.00	46.48
	1633	O	HOH	A	15	23.871	76.354	23.810	1.00	36.55
	1634	O	HOH	A	16	28.656	78.595	14.195	1.00	48.95
	1635	O	HOH	A	17	26.439	59.235	16.698	1.00	50.90
	1636	O	HOH	A	18	48.822	76.573	10.696	1.00	58.83
45	1637	O	HOH	A	19	46.016	72.983	15.254	1.00	61.24
	1638	O	HOH	A	20	18.011	59.153	0.608	1.00	58.37
	1639	O	HOH	A	21	10.586	67.712	6.227	1.00	57.48
	1640	O	HOH	A	22	39.217	50.176	20.140	1.00	60.62
	1641	O	HOH	A	23	19.990	55.647	11.936	1.00	49.14
50	1642	O	HOH	A	24	18.092	104.938	6.774	1.00	63.67
	1643	O	HOH	A	25	11.413	86.589	17.509	1.00	40.50
	1644	O	HOH	A	26	55.940	62.358	0.863	1.00	58.12
	1645	O	HOH	A	27	26.856	64.971	15.189	1.00	52.34
	1646	O	HOH	A	28	32.914	64.797	12.453	1.00	52.41
55	1647	O	HOH	A	29	23.938	107.034	22.326	1.00	63.47

	1648	O	HOH	A	30	28.142	76.042	14.972	1.00	56.91
	1649	O	HOH	A	31	34.884	65.010	3.193	1.00	49.06
	1650	O	HOH	A	32	10.166	82.530	4.732	1.00	59.31
	1651	O	HOH	A	33	28.781	47.212	5.405	1.00	51.40
5	1652	O	HOH	A	34	26.373	54.646	2.184	1.00	49.71
	1653	O	HOH	A	35	50.871	71.532	11.654	1.00	64.98
	1654	O	HOH	A	36	14.970	75.672	2.416	1.00	55.97
	1655	O	HOH	A	37	7.183	75.882	18.351	1.00	56.10
	1656	O	HOH	A	38	8.889	71.461	23.144	1.00	48.69
10	1657	O	HOH	A	39	16.590	67.594	29.822	1.00	58.57
	1658	O	HOH	A	40	38.458	52.685	18.905	1.00	54.81
	1659	O	HOH	A	41	54.406	64.045	8.519	1.00	65.02
	1660	O	HOH	A	42	10.751	53.102	5.496	1.00	60.95
	1661	O	HOH	A	43	52.001	82.188	9.439	1.00	59.29
15	1662	O	HOH	A	44	16.985	77.359	2.354	1.00	64.70
	1663	O	HOH	A	45	20.295	50.729	1.374	1.00	57.91
	1664	O	HOH	A	46	23.952	95.782	3.814	1.00	54.20
	1665	O	HOH	A	47	14.130	79.241	2.012	1.00	59.40
	1666	O	HOH	A	48	42.373	77.528	8.231	1.00	61.07
20	1667	O	HOH	A	49	49.811	60.323	14.343	1.00	62.77
	1668	O	HOH	A	50	32.587	60.842	17.597	1.00	54.90
	1669	O	HOH	A	51	26.700	67.334	3.009	1.00	59.03
	1670	O	HOH	A	52	27.137	97.388	12.542	1.00	57.55
	1671	O	HOH	A	53	19.726	104.219	18.295	1.00	55.02
25	1672	O	HOH	A	54	27.571	78.794	11.807	1.00	62.62
	1673	O	HOH	A	55	10.438	93.153	21.642	1.00	64.18
	1674	O	HOH	A	56	20.189	101.789	21.921	1.00	57.80
	1675	O	HOH	A	57	45.236	75.729	14.048	1.00	68.28
	1676	O	HOH	A	58	28.726	86.130	15.755	1.00	42.77
30	1677	O	HOH	A	59	15.761	61.916	22.864	1.00	49.12
	1678	O	HOH	A	60	18.673	97.101	18.412	1.00	60.00
	1679	O	HOH	A	61	51.586	62.841	8.977	1.00	66.82
	1680	O	HOH	A	62	12.665	48.318	9.830	1.00	61.58
	1681	O	HOH	A	63	10.994	69.841	26.147	1.00	54.56
35	1682	O	HOH	A	64	34.004	50.096	9.090	1.00	52.20
	1683	O	HOH	A	65	22.928	54.076	3.637	1.00	63.55
	1684	O	HOH	A	66	13.124	80.438	22.463	1.00	49.41
	1685	O	HOH	A	67	14.496	84.734	-3.782	1.00	59.74
	1686	O	HOH	A	68	33.203	84.033	9.037	1.00	61.59
40	1687	O	HOH	A	69	25.151	70.683	28.546	1.00	58.32
	1688	O	HOH	A	70	43.528	47.541	7.082	1.00	67.46
	1689	O	HOH	A	71	28.976	58.922	-3.873	1.00	56.29
	1690	O	HOH	A	72	39.085	57.630	3.442	1.00	57.89
	1691	O	HOH	A	73	34.708	46.624	11.157	1.00	61.84
45	1692	O	HOH	A	74	3.300	67.675	10.833	1.00	70.53
	1693	O	HOH	A	75	23.591	70.505	16.477	1.00	53.22
	1694	O	HOH	A	76	15.993	56.650	1.105	1.00	60.73
	1695	O	HOH	A	77	51.586	54.551	5.644	1.00	64.35
	1696	O	HOH	A	78	14.626	95.986	18.718	1.00	59.27
50	1697	O	HOH	A	79	23.734	74.708	12.176	1.00	53.70
	1698	O	HOH	A	80	17.100	96.977	3.795	1.00	60.32
	1699	O	HOH	A	81	9.533	67.755	26.736	1.00	56.40
	1700	O	HOH	A	82	18.888	66.846	28.479	1.00	62.11
	1701	O	HOH	A	83	43.839	71.746	16.116	1.00	57.66
55	1702	O	HOH	A	84	8.517	74.508	22.311	1.00	61.70
	1703	O	HOH	A	85	41.870	49.996	21.891	1.00	61.38
	1704	O	HOH	A	86	14.562	94.919	2.718	1.00	67.86
	1705	O	HOH	A	87	28.791	96.969	19.836	1.00	61.99
	1706	O	HOH	A	88	23.437	78.234	7.551	1.00	54.45
5	1707	O	HOH	A	89	29.614	80.314	4.323	1.00	57.86
	1708	O	HOH	A	90	28.546	67.893	5.438	1.00	58.43
	1709	O	HOH	A	91	47.040	72.908	13.045	1.00	67.78

	1710	O	HOH	A	92	42.407	51.656	18.123	1.00	65.22
	1711	O	HOH	A	93	23.749	65.735	-2.072	1.00	60.31
	1712	O	HOH	A	94	44.018	74.292	16.194	1.00	61.54
	1713	O	HOH	A	95	11.601	46.086	10.312	1.00	67.64
	1714	O	HOH	A	96	6.175	66.153	17.508	1.00	56.59
	1715	O	HOH	A	97	31.504	47.151	3.997	1.00	64.62
	1716	O	HOH	A	98	42.312	75.926	6.322	1.00	66.03
	1717	O	HOH	A	99	31.022	57.142	18.155	1.00	62.65
	1718	O	HOH	A	100	17.995	104.383	3.752	1.00	63.95
	1719	O	HOH	A	101	10.716	86.701	-4.491	1.00	63.86
	1720	O	HOH	A	102	27.763	72.631	16.379	1.00	62.58
	1721	O	HOH	A	103	15.381	105.037	7.270	1.00	58.40
	1722	O	HOH	A	104	47.651	78.799	15.518	1.00	61.34
	1723	O	HOH	A	105	34.927	94.559	9.949	1.00	65.87
	1724	O	HOH	A	106	9.087	82.761	20.779	1.00	61.27
	1725	O	HOH	A	107	22.682	53.866	0.739	1.00	67.17
	1726	O	HOH	A	108	37.349	58.563	-1.263	1.00	54.90
	1727	O	HOH	A	109	24.982	97.874	2.783	1.00	66.23
	1728	O	HOH	A	110	31.881	73.012	28.973	1.00	59.96
	1729	O	HOH	A	111	47.953	60.989	1.790	1.00	64.92
	1730	O	HOH	A	112	42.129	73.312	10.101	1.00	65.68
	1731	O	HOH	A	113	36.875	58.541	1.642	1.00	61.47
	1732	O	HOH	A	114	35.326	52.952	2.865	1.00	60.20
	1733	O	HOH	A	115	6.136	77.374	20.212	1.00	59.29
	1734	O	HOH	A	116	25.741	94.929	18.879	1.00	53.05
	1735	O	HOH	A	117	54.362	58.376	9.533	1.00	69.15
	1736	O	HOH	A	118	23.326	103.523	17.163	1.00	62.28
	1737	O	HOH	A	119	5.978	83.975	15.596	1.00	59.61
	1738	O	HOH	A	120	33.072	54.315	0.721	1.00	61.94
	1739	O	HOH	A	121	37.197	45.372	11.843	1.00	64.45
	1740	O	HOH	A	122	11.834	65.339	3.962	1.00	63.01
	1741	O	HOH	A	123	16.132	79.865	0.613	1.00	59.29
	1742	O	HOH	A	124	12.804	74.215	0.796	1.00	61.69
	1743	O	HOH	A	125	6.166	72.199	12.094	1.00	69.10
	1744	O	HOH	A	126	46.672	51.916	3.111	1.00	61.79
	1745	O	HOH	A	127	21.940	56.684	-1.243	1.00	63.74
	1746	O	HOH	A	128	19.803	72.626	40.522	1.00	67.04
	1747	O	HOH	A	129	28.002	103.109	11.797	1.00	62.20
	1748	O	HOH	A	130	16.264	66.529	27.554	1.00	66.48
	1749	O	HOH	A	131	38.684	71.694	5.498	1.00	70.79
	1750	O	HOH	A	132	30.875	98.591	19.410	1.00	72.41
	1751	O	HOH	A	133	20.444	64.387	22.091	1.00	62.09
	1752	O	HOH	A	134	16.959	52.193	1.564	1.00	61.32
	1753	O	HOH	A	135	43.707	44.495	7.969	1.00	68.49
	1754	O	HOH	A	136	27.297	51.198	-3.047	1.00	69.04
	1755	O	HOH	A	137	45.002	47.522	9.091	1.00	63.49
	1756	O	HOH	A	138	20.670	82.001	-0.631	1.00	53.37
	1757	O	HOH	A	139	18.747	100.351	20.086	1.00	59.07
	1758	O	HOH	A	140	43.001	46.804	15.782	1.00	65.35
	1759	O	HOH	A	141	56.594	54.897	10.204	1.00	67.74
	1760	O	HOH	A	142	16.980	94.578	0.460	1.00	67.40
	1761	O	HOH	A	143	34.493	68.011	5.655	1.00	64.43
	1762	O	HOH	A	144	7.561	88.413	-1.394	1.00	67.27
	1763	O	HOH	A	145	55.370	75.436	6.692	1.00	70.07
	1764	N	VAL	B	336	42.982	59.443	29.109	1.00	58.93
	1765	CA	VAL	B	336	43.788	60.200	30.107	1.00	60.44
	1766	C	VAL	B	336	44.173	61.587	29.599	1.00	60.07
	1767	O	VAL	B	336	45.211	61.753	28.958	1.00	61.48
	1768	CB	VAL	B	336	45.079	59.445	30.453	1.00	60.81
	1769	CG1	VAL	B	336	45.794	60.136	31.600	1.00	61.71
	1770	CG2	VAL	B	336	44.755	58.010	30.798	1.00	64.73
	1771	N	SER	B	337	43.343	62.583	29.891	1.00	57.95

	1772	CA	SER	B	337	43.617	63.945	29.452	1.00	56.60
	1773	C	SER	B	337	43.758	64.917	30.624	1.00	55.17
	1774	O	SER	B	337	43.338	64.619	31.748	1.00	54.55
	1775	CB	SER	B	337	42.522	64.415	28.497	1.00	57.92
	1776	OG	SER	B	337	41.244	64.111	29.013	1.00	64.70
	1777	N	ALA	B	338	44.362	66.073	30.357	1.00	52.40
	1778	CA	ALA	B	338	44.590	67.078	31.389	1.00	50.69
	1779	C	ALA	B	338	44.300	68.491	30.908	1.00	50.25
	1780	O	ALA	B	338	44.538	68.828	29.746	1.00	51.17
	1781	CB	ALA	B	338	46.027	66.989	31.889	1.00	50.21
	1782	N	TYR	B	339	43.792	69.319	31.816	1.00	48.22
	1783	CA	TYR	B	339	43.461	70.701	31.495	1.00	46.82
	1784	C	TYR	B	339	43.834	71.610	32.669	1.00	44.51
	1785	O	TYR	B	339	43.711	71.228	33.832	1.00	42.27
	1786	CB	TYR	B	339	41.962	70.835	31.185	1.00	50.52
	1787	CG	TYR	B	339	41.402	69.731	30.307	1.00	58.40
	1788	CD1	TYR	B	339	41.155	68.456	30.826	1.00	61.23
	1789	CD2	TYR	B	339	41.144	69.952	28.949	1.00	60.99
	1790	CE1	TYR	B	339	40.671	67.426	30.019	1.00	62.71
	1791	CE2	TYR	B	339	40.657	68.926	28.131	1.00	63.53
	1792	CZ	TYR	B	339	40.424	67.667	28.673	1.00	64.33
	1793	OH	TYR	B	339	39.956	66.647	27.870	1.00	65.07
	1794	N	LEU	B	340	44.309	72.807	32.354	1.00	41.90
	1795	CA	LEU	B	340	44.695	73.769	33.372	1.00	41.06
	1796	C	LEU	B	340	43.929	75.029	33.022	1.00	41.10
	1797	O	LEU	B	340	43.953	75.464	31.876	1.00	43.45
	1798	CB	LEU	B	340	46.208	74.017	33.321	1.00	36.93
	1799	CG	LEU	B	340	46.830	74.911	34.399	1.00	35.91
	1800	CD1	LEU	B	340	46.500	74.371	35.786	1.00	34.60
	1801	CD2	LEU	B	340	48.336	74.979	34.194	1.00	35.51
	1802	N	SER	B	341	43.232	75.610	33.992	1.00	39.82
	1803	CA	SER	B	341	42.448	76.810	33.715	1.00	39.85
	1804	C	SER	B	341	42.955	78.002	34.486	1.00	37.88
	1805	O	SER	B	341	43.524	77.863	35.556	1.00	42.10
	1806	CB	SER	B	341	40.973	76.575	34.058	1.00	39.34
	1807	OG	SER	B	341	40.808	76.253	35.428	1.00	44.58
	1808	N	ARG	B	342	42.732	79.185	33.942	1.00	36.98
	1809	CA	ARG	B	342	43.163	80.413	34.583	1.00	35.20
	1810	C	ARG	B	342	42.183	80.747	35.707	1.00	33.18
	1811	O	ARG	B	342	41.157	80.092	35.848	1.00	33.16
	1812	CB	ARG	B	342	43.206	81.530	33.534	1.00	38.57
	1813	CG	ARG	B	342	44.219	81.279	32.411	1.00	39.10
	1814	CD	ARG	B	342	44.236	82.409	31.388	1.00	43.21
	1815	NE	ARG	B	342	43.056	82.369	30.530	1.00	45.40
	1816	CZ	ARG	B	342	42.886	81.514	29.527	1.00	48.22
	1817	NH1	ARG	B	342	43.823	80.623	29.240	1.00	52.78
	1818	NH2	ARG	B	342	41.769	81.541	28.814	1.00	54.34
	1819	N	PRO	B	343	42.488	81.757	36.530	1.00	33.03
	1820	CA	PRO	B	343	41.560	82.103	37.619	1.00	34.14
	1821	C	PRO	B	343	40.261	82.693	37.065	1.00	34.06
	1822	O	PRO	B	343	40.259	83.298	35.994	1.00	35.44
	1823	CB	PRO	B	343	42.334	83.152	38.433	1.00	33.07
	1824	CG	PRO	B	343	43.789	82.900	38.075	1.00	35.06
	1825	CD	PRO	B	343	43.715	82.571	36.601	1.00	33.27
	1826	N	SER	B	344	39.155	82.520	37.775	1.00	32.17
	1827	CA	SER	B	344	37.909	83.110	37.308	1.00	31.75
	1828	C	SER	B	344	37.983	84.586	37.686	1.00	32.07
	1829	O	SER	B	344	38.485	84.940	38.756	1.00	30.21
	1830	CB	SER	B	344	36.693	82.456	37.982	1.00	32.20
	1831	OG	SER	B	344	36.487	82.935	39.301	1.00	32.50
	1832	N	PRO	B	345	37.512	85.473	36.800	1.00	32.31
	1833	CA	PRO	B	345	37.561	86.899	37.125	1.00	30.84

1834	C	PRO	B	345	36.890	87.219	38.471	1.00	29.64
1835	O	PRO	B	345	37.344	88.094	39.209	1.00	30.14
1836	CB	PRO	B	345	36.859	87.545	35.926	1.00	30.96
1837	CG	PRO	B	345	37.299	86.659	34.793	1.00	33.18
1838	CD	PRO	B	345	37.143	85.261	35.387	1.00	33.65
1839	N	PHE	B	346	35.831	86.497	38.808	1.00	28.34
1840	CA	PHE	B	346	35.153	86.756	40.066	1.00	31.46
1841	C	PHE	B	346	36.078	86.515	41.269	1.00	32.46
1842	O	PHE	B	346	36.135	87.331	42.193	1.00	32.59
1843	CB	PHE	B	346	33.894	85.889	40.184	1.00	32.72
1844	CG	PHE	B	346	33.218	85.987	41.521	1.00	36.34
1845	CD1	PHE	B	346	32.619	87.170	41.928	1.00	40.58
1846	CD2	PHE	B	346	33.189	84.898	42.378	1.00	36.76
1847	CE1	PHE	B	346	31.991	87.267	43.167	1.00	38.98
1848	CE2	PHE	B	346	32.563	84.985	43.618	1.00	40.15
1849	CZ	PHE	B	346	31.963	86.175	44.014	1.00	38.60
1850	N	ASP	B	347	36.803	85.397	41.250	1.00	32.92
1851	CA	ASP	B	347	37.723	85.066	42.336	1.00	33.58
1852	C	ASP	B	347	38.896	86.045	42.367	1.00	34.26
1853	O	ASP	B	347	39.388	86.408	43.434	1.00	32.29
1854	CB	ASP	B	347	38.251	83.633	42.179	1.00	28.72
1855	CG	ASP	B	347	37.236	82.592	42.579	1.00	39.62
1856	OD1	ASP	B	347	37.515	81.375	42.429	1.00	42.08
1857	OD2	ASP	B	347	36.151	82.991	43.054	1.00	46.23
1858	N	LEU	B	348	39.324	86.480	41.189	1.00	34.31
1859	CA	LEU	B	348	40.441	87.403	41.064	1.00	37.70
1860	C	LEU	B	348	40.159	88.858	41.471	1.00	38.98
1861	O	LEU	B	348	40.949	89.463	42.198	1.00	38.11
1862	CB	LEU	B	348	40.959	87.380	39.618	1.00	40.66
1863	CG	LEU	B	348	42.159	88.267	39.260	1.00	41.99
1864	CD1	LEU	B	348	43.388	87.862	40.095	1.00	42.77
1865	CD2	LEU	B	348	42.469	88.124	37.759	1.00	41.00
1866	N	PHE	B	349	39.040	89.417	41.017	1.00	39.68
1867	CA	PHE	B	349	38.725	90.819	41.306	1.00	42.09
1868	C	PHE	B	349	37.717	91.134	42.405	1.00	45.09
1869	O	PHE	B	349	37.821	92.169	43.062	1.00	48.27
1870	CB	PHE	B	349	38.272	91.526	40.029	1.00	37.36
1871	CG	PHE	B	349	39.244	91.411	38.900	1.00	36.93
1872	CD1	PHE	B	349	38.976	90.579	37.818	1.00	38.16
1873	CD2	PHE	B	349	40.444	92.113	38.926	1.00	38.04
1874	CE1	PHE	B	349	39.885	90.445	36.781	1.00	38.11
1875	CE2	PHE	B	349	41.369	91.986	37.887	1.00	37.58
1876	CZ	PHE	B	349	41.089	91.151	36.817	1.00	40.39
1877	N	ILE	B	350	36.726	90.277	42.600	1.00	46.66
1878	CA	ILE	B	350	35.746	90.548	43.639	1.00	48.94
1879	C	ILE	B	350	36.200	89.905	44.950	1.00	51.15
1880	O	ILE	B	350	36.505	90.593	45.921	1.00	50.51
1881	CB	ILE	B	350	34.359	90.008	43.240	1.00	48.52
1882	CG1	ILE	B	350	34.038	90.428	41.801	1.00	49.25
1883	CG2	ILE	B	350	33.300	90.548	44.177	1.00	49.68
1884	CD1	ILE	B	350	34.242	91.911	41.533	1.00	46.80
1885	N	ARG	B	351	36.265	88.579	44.945	1.00	52.64
1886	CA	ARG	B	351	36.669	87.793	46.100	1.00	53.76
1887	C	ARG	B	351	38.114	88.090	46.519	1.00	53.61
1888	O	ARG	B	351	38.436	88.094	47.703	1.00	53.55
1889	CB	ARG	B	351	36.505	86.313	45.759	1.00	56.64
1890	CG	ARG	B	351	36.016	85.434	46.894	1.00	62.18
1891	CD	ARG	B	351	35.073	84.375	46.348	1.00	66.96
1892	NE	ARG	B	351	34.958	83.211	47.219	1.00	71.13
1893	CZ	ARG	B	351	35.957	82.371	47.470	1.00	76.72
1894	NH1	ARG	B	351	37.145	82.573	46.916	1.00	78.73
1895	NH2	ARG	B	351	35.771	81.325	48.268	1.00	77.63

	1896	N	LYS	B	352	38.974	88.347	45.540	1.00	53.86
	1897	CA	LYS	B	352	40.385	88.646	45.788	1.00	54.12
	1898	C	LYS	B	352	41.172	87.449	46.328	1.00	52.02
	1899	O	LYS	B	352	42.078	87.604	47.146	1.00	51.77
	1900	CB	LYS	B	352	40.525	89.825	46.753	1.00	57.77
	1901	CG	LYS	B	352	39.911	91.124	46.254	1.00	62.15
	1902	CD	LYS	B	352	40.161	92.252	47.254	1.00	71.06
	1903	CE	LYS	B	352	39.351	93.502	46.929	1.00	74.25
	1904	NZ	LYS	B	352	37.893	93.307	47.185	1.00	78.35
	1905	N	SER	B	353	40.811	86.258	45.867	1.00	48.01
	1906	CA	SER	B	353	41.488	85.032	46.268	1.00	45.29
	1907	C	SER	B	353	41.446	84.056	45.084	1.00	40.67
	1908	O	SER	B	353	40.725	83.054	45.106	1.00	40.76
	1909	CB	SER	B	353	40.809	84.423	47.498	1.00	47.97
	1910	OG	SER	B	353	39.445	84.152	47.247	1.00	56.20
	1911	N	PRO	B	354	42.225	84.356	44.030	1.00	36.53
	1912	CA	PRO	B	354	42.361	83.596	42.781	1.00	32.68
	1913	C	PRO	B	354	42.940	82.201	42.961	1.00	31.88
	1914	O	PRO	B	354	43.813	81.985	43.798	1.00	29.76
	1915	CB	PRO	B	354	43.306	84.453	41.940	1.00	30.29
	1916	CG	PRO	B	354	43.260	85.801	42.587	1.00	41.68
	1917	CD	PRO	B	354	43.155	85.494	44.035	1.00	33.29
	1918	N	THR	B	355	42.446	81.258	42.168	1.00	30.03
	1919	CA	THR	B	355	42.956	79.896	42.198	1.00	29.70
	1920	C	THR	B	355	43.022	79.364	40.774	1.00	30.82
	1921	O	THR	B	355	42.302	79.827	39.887	1.00	30.67
	1922	CB	THR	B	355	42.042	78.931	42.964	1.00	32.14
	1923	OG1	THR	B	355	40.815	78.794	42.240	1.00	29.97
	1924	CG2	THR	B	355	41.763	79.425	44.393	1.00	31.76
	1925	N	ILE	B	356	43.907	78.405	40.542	1.00	30.53
	1926	CA	ILE	B	356	43.969	77.784	39.232	1.00	31.56
	1927	C	ILE	B	356	43.740	76.321	39.525	1.00	31.79
	1928	O	ILE	B	356	44.039	75.848	40.625	1.00	30.35
	1929	CB	ILE	B	356	45.315	78.016	38.517	1.00	30.05
	1930	CG1	ILE	B	356	46.467	77.499	39.371	1.00	31.32
	1931	CG2	ILE	B	356	45.469	79.508	38.210	1.00	31.27
	1932	CD1	ILE	B	356	47.828	77.757	38.763	1.00	36.89
	1933	N	THR	B	357	43.198	75.605	38.550	1.00	33.31
	1934	CA	THR	B	357	42.881	74.205	38.751	1.00	33.68
	1935	C	THR	B	357	43.403	73.318	37.644	1.00	35.47
	1936	O	THR	B	357	43.228	73.607	36.459	1.00	36.65
	1937	CB	THR	B	357	41.335	74.011	38.855	1.00	33.81
	1938	OG1	THR	B	357	40.844	74.683	40.023	1.00	33.71
	1939	CG2	THR	B	357	40.968	72.535	38.921	1.00	29.63
	1940	N	CYS	B	358	44.034	72.228	38.048	1.00	35.41
	1941	CA	CYS	B	358	44.561	71.254	37.110	1.00	38.12
	1942	C	CYS	B	358	43.570	70.093	37.165	1.00	37.77
	1943	O	CYS	B	358	43.395	69.473	38.210	1.00	36.67
	1944	CB	CYS	B	358	45.945	70.789	37.568	1.00	40.37
	1945	SG	CYS	B	358	46.871	69.769	36.374	1.00	49.83
	1946	N	LEU	B	359	42.909	69.822	36.046	1.00	39.77
	1947	CA	LEU	B	359	41.932	68.747	35.973	1.00	42.86
	1948	C	LEU	B	359	42.432	67.593	35.123	1.00	46.01
	1949	O	LEU	B	359	42.748	67.769	33.948	1.00	47.43
	1950	CB	LEU	B	359	40.612	69.265	35.389	1.00	42.74
	1951	CG	LEU	B	359	39.604	68.208	34.904	1.00	45.03
	1952	CD1	LEU	B	359	39.152	67.338	36.057	1.00	47.59
	1953	CD2	LEU	B	359	38.403	68.889	34.262	1.00	47.51
	1954	N	VAL	B	360	42.493	66.411	35.721	1.00	48.26
	1955	CA	VAL	B	360	42.931	65.220	35.010	1.00	52.34
	1956	C	VAL	B	360	41.765	64.243	34.883	1.00	55.48
	1957	O	VAL	B	360	41.092	63.928	35.866	1.00	55.57

	1958	CB	VAL	B	360	44.100	64.527	35.747	1.00	53.36
	1959	CG1	VAL	B	360	44.481	63.240	35.029	1.00	51.62
	1960	CG2	VAL	B	360	45.299	65.467	35.816	1.00	51.77
	1961	N	VAL	B	361	41.520	63.773	33.665	1.00	58.92
	1962	CA	VAL	B	361	40.433	62.834	33.416	1.00	63.13
	1963	C	VAL	B	361	40.993	61.506	32.926	1.00	67.77
	1964	O	VAL	B	361	41.738	61.466	31.946	1.00	68.38
	1965	CB	VAL	B	361	39.442	63.377	32.353	1.00	60.50
	1966	CG1	VAL	B	361	38.358	62.355	32.086	1.00	56.92
	1967	CG2	VAL	B	361	38.814	64.671	32.830	1.00	56.10
	1968	N	ASP	B	362	40.635	60.426	33.615	1.00	72.90
	1969	CA	ASP	B	362	41.098	59.085	33.259	1.00	78.30
	1970	C	ASP	B	362	39.904	58.244	32.816	1.00	81.68
	1971	O	ASP	B	362	39.168	57.709	33.648	1.00	81.72
	1972	CB	ASP	B	362	41.771	58.415	34.462	1.00	80.22
	1973	CG	ASP	B	362	42.530	57.156	34.080	1.00	84.67
	1974	OD1	ASP	B	362	42.113	56.478	33.117	1.00	87.54
	1975	OD2	ASP	B	362	43.537	56.837	34.749	1.00	87.19
	1976	N	LEU	B	363	39.723	58.126	31.503	1.00	85.84
	1977	CA	LEU	B	363	38.614	57.366	30.935	1.00	89.95
	1978	C	LEU	B	363	38.562	55.923	31.428	1.00	92.20
	1979	O	LEU	B	363	37.483	55.386	31.668	1.00	92.55
	1980	CB	LEU	B	363	38.694	57.390	29.409	1.00	91.66
	1981	CG	LEU	B	363	38.719	58.777	28.758	1.00	92.93
	1982	CD1	LEU	B	363	38.813	58.624	27.246	1.00	95.41
	1983	CD2	LEU	B	363	37.471	59.551	29.137	1.00	92.73
	1984	N	ALA	B	364	39.726	55.296	31.573	1.00	94.76
	1985	CA	ALA	B	364	39.801	53.916	32.051	1.00	97.66
	1986	C	ALA	B	364	40.794	53.831	33.210	1.00	99.72
	1987	O	ALA	B	364	41.998	53.996	33.021	1.00	100.44
	1988	CB	ALA	B	364	40.235	52.996	30.921	1.00	97.99
	1989	N	PRO	B	365	40.297	53.577	34.429	1.00	101.15
	1990	CA	PRO	B	365	41.173	53.484	35.602	1.00	102.25
	1991	C	PRO	B	365	41.895	52.163	35.855	1.00	103.43
	1992	O	PRO	B	365	41.274	51.103	35.934	1.00	104.19
	1993	CB	PRO	B	365	40.237	53.829	36.761	1.00	101.91
	1994	CG	PRO	B	365	39.121	54.617	36.098	1.00	102.27
	1995	CD	PRO	B	365	38.910	53.833	34.846	1.00	101.40
	1996	N	SER	B	366	43.215	52.256	35.979	1.00	104.18
	1997	CA	SER	B	366	44.088	51.132	36.299	1.00	104.43
	1998	C	SER	B	366	44.573	51.676	37.637	1.00	104.05
	1999	O	SER	B	366	44.888	52.864	37.727	1.00	104.36
	2000	CB	SER	B	366	45.249	51.055	35.312	1.00	105.50
	2001	OG	SER	B	366	46.040	52.223	35.413	1.00	106.70
	2002	N	LYS	B	367	44.645	50.861	38.682	1.00	103.19
	2003	CA	LYS	B	367	45.041	51.462	39.944	1.00	102.08
	2004	C	LYS	B	367	46.491	51.630	40.367	1.00	100.74
	2005	O	LYS	B	367	47.234	50.683	40.640	1.00	101.05
	2006	CB	LYS	B	367	44.236	50.868	41.102	1.00	103.30
	2007	CG	LYS	B	367	44.343	49.384	41.345	1.00	105.00
	2008	CD	LYS	B	367	43.374	49.046	42.467	1.00	104.80
	2009	CE	LYS	B	367	43.467	47.610	42.930	1.00	104.70
	2010	NZ	LYS	B	367	42.524	47.386	44.066	1.00	105.18
	2011	N	GLY	B	368	46.839	52.909	40.422	1.00	98.70
	2012	CA	GLY	B	368	48.136	53.408	40.828	1.00	95.62
	2013	C	GLY	B	368	47.700	54.801	41.244	1.00	93.12
	2014	O	GLY	B	368	46.538	55.143	41.035	1.00	93.17
	2015	N	THR	B	369	48.569	55.617	41.823	1.00	90.15
	2016	CA	THR	B	369	48.125	56.948	42.220	1.00	86.41
	2017	C	THR	B	369	48.420	57.977	41.136	1.00	83.04
	2018	O	THR	B	369	49.402	57.854	40.401	1.00	82.54
	2019	CB	THR	B	369	48.792	57.397	43.541	1.00	87.73

	2020	OG1	THR	B	369	50.217	57.422	43.379	1.00	88.60
	2021	CG2	THR	B	369	48.423	56.443	44.671	1.00	86.64
45	2022	N	VAL	B	370	47.552	58.980	41.027	1.00	79.07
	2023	CA	VAL	B	370	47.729	60.041	40.042	1.00	74.46
	2024	C	VAL	B	370	48.275	61.261	40.768	1.00	72.21
	2025	O	VAL	B	370	47.602	61.838	41.618	1.00	71.35
	2026	CB	VAL	B	370	46.401	60.420	39.368	1.00	73.33
50	2027	CG1	VAL	B	370	46.667	61.346	38.196	1.00	70.92
	2028	CG2	VAL	B	370	45.674	59.173	38.915	1.00	69.77
	2029	N	ASN	B	371	49.498	61.653	40.426	1.00	70.13
	2030	CA	ASN	B	371	50.137	62.791	41.073	1.00	68.15
	2031	C	ASN	B	371	50.157	64.079	40.262	1.00	65.65
55	2032	O	ASN	B	371	50.352	64.067	39.046	1.00	64.64

	2033	CB	ASN	B	371	51.564	62.421	41.469	1.00	70.12
	2034	CG	ASN	B	371	51.605	61.330	42.508	1.00	73.56
	2035	OD1	ASN	B	371	51.153	61.519	43.638	1.00	75.10
	2036	ND2	ASN	B	371	52.137	60.173	42.131	1.00	74.76
5	2037	N	LEU	B	372	49.949	65.192	40.959	1.00	62.66
	2038	CA	LEU	B	372	49.959	66.512	40.346	1.00	59.53
	2039	C	LEU	B	372	50.927	67.374	41.137	1.00	56.68
	2040	O	LEU	B	372	50.788	67.529	42.347	1.00	56.70
	2041	CB	LEU	B	372	48.560	67.141	40.372	1.00	59.44
10	2042	CG	LEU	B	372	47.428	66.383	39.678	1.00	60.55
	2043	CD1	LEU	B	372	46.214	67.277	39.579	1.00	61.28
	2044	CD2	LEU	B	372	47.861	65.956	38.293	1.00	62.83
	2045	N	THR	B	373	51.911	67.931	40.446	1.00	53.76
	2046	CA	THR	B	373	52.915	68.766	41.085	1.00	51.64
15	2047	C	THR	B	373	52.850	70.180	40.512	1.00	48.20
	2048	O	THR	B	373	52.801	70.355	39.296	1.00	46.65
	2049	CB	THR	B	373	54.325	68.201	40.832	1.00	53.15
	2050	OG1	THR	B	373	54.324	66.789	41.073	1.00	57.77
	2051	CG2	THR	B	373	55.339	68.871	41.747	1.00	53.75
20	2052	N	TRP	B	374	52.851	71.181	41.385	1.00	45.34
	2053	CA	TRP	B	374	52.799	72.575	40.942	1.00	44.94
	2054	C	TRP	B	374	54.161	73.259	41.041	1.00	43.68
	2055	O	TRP	B	374	54.945	72.964	41.938	1.00	42.67
	2056	CB	TRP	B	374	51.805	73.391	41.784	1.00	41.63
25	2057	CG	TRP	B	374	50.371	72.977	41.657	1.00	41.50
	2058	CD1	TRP	B	374	49.688	72.124	42.477	1.00	39.67
	2059	CD2	TRP	B	374	49.441	73.395	40.648	1.00	35.69
	2060	NE1	TRP	B	374	48.392	71.988	42.041	1.00	35.06
	2061	CE2	TRP	B	374	48.214	72.756	40.922	1.00	34.53
30	2062	CE3	TRP	B	374	49.528	74.247	39.542	1.00	32.37
	2063	CZ2	TRP	B	374	47.079	72.943	40.129	1.00	35.43
	2064	CZ3	TRP	B	374	48.401	74.434	38.751	1.00	36.11
	2065	CH2	TRP	B	374	47.190	73.782	39.050	1.00	37.51
	2066	N	SER	B	375	54.430	74.179	40.119	1.00	43.53
35	2067	CA	SER	B	375	55.678	74.934	40.140	1.00	43.57
	2068	C	SER	B	375	55.511	76.270	39.438	1.00	42.59
	2069	O	SER	B	375	54.669	76.411	38.550	1.00	43.68
	2070	CB	SER	B	375	56.820	74.153	39.474	1.00	45.03
	2071	OG	SER	B	375	56.691	74.118	38.066	1.00	45.66
40	2072	N	ARG	B	376	56.299	77.251	39.866	1.00	40.79
	2073	CA	ARG	B	376	56.279	78.569	39.266	1.00	40.12
	2074	C	ARG	B	376	57.498	78.689	38.351	1.00	40.59
	2075	O	ARG	B	376	58.618	78.393	38.752	1.00	40.90
	2076	CB	ARG	B	376	56.345	79.653	40.334	1.00	40.03
45	2077	CG	ARG	B	376	55.132	79.745	41.237	1.00	43.20
	2078	CD	ARG	B	376	54.883	81.198	41.599	1.00	41.05
	2079	NE	ARG	B	376	55.171	81.480	42.992	1.00	50.71
	2080	CZ	ARG	B	376	55.300	82.705	43.488	1.00	53.97
	2081	NH1	ARG	B	376	55.172	83.758	42.693	1.00	51.88

	2082	NH2	ARG	B	376	55.542	82.874	44.782	1.00	55.55
	2083	N	ALA	B	377	57.281	79.129	37.122	1.00	40.20
	2084	CA	ALA	B	377	58.382	79.273	36.181	1.00	40.25
	2085	C	ALA	B	377	59.500	80.130	36.786	1.00	40.38
	2086	O	ALA	B	377	60.657	79.979	36.422	1.00	41.16
	2087	CB	ALA	B	377	57.879	79.903	34.878	1.00	33.12
	2088	N	SER	B	378	59.144	81.015	37.714	1.00	40.21
	2089	CA	SER	B	378	60.109	81.903	38.354	1.00	41.95
	2090	C	SER	B	378	60.906	81.188	39.436	1.00	44.92
	2091	O	SER	B	378	61.866	81.744	39.966	1.00	44.28
	2092	CB	SER	B	378	59.401	83.096	38.992	1.00	40.91
	2093	OG	SER	B	378	58.737	82.693	40.180	1.00	40.09
	2094	N	GLY	B	379	60.493	79.967	39.768	1.00	46.93
	2095	CA	GLY	B	379	61.181	79.195	40.787	1.00	49.77
	2096	C	GLY	B	379	60.716	79.512	42.196	1.00	50.60
	2097	O	GLY	B	379	61.024	78.783	43.142	1.00	52.95
	2098	N	LYS	B	380	59.974	80.605	42.345	1.00	53.72
	2099	CA	LYS	B	380	59.478	80.988	43.657	1.00	54.13
	2100	C	LYS	B	380	58.564	79.911	44.255	1.00	48.16
	2101	O	LYS	B	380	58.087	79.008	43.556	1.00	45.65
	2102	CB	LYS	B	380	58.752	82.338	43.583	1.00	62.44
	2103	CG	LYS	B	380	59.692	83.522	43.390	1.00	67.72
	2104	CD	LYS	B	380	58.975	84.852	43.550	1.00	69.32
	2105	CE	LYS	B	380	59.956	86.013	43.481	1.00	73.14
	2106	NZ	LYS	B	380	59.280	87.333	43.633	1.00	77.37
	2107	N	PRO	B	381	58.323	79.986	45.571	1.00	56.07
	2108	CA	PRO	B	381	57.472	79.014	46.265	1.00	56.46
	2109	C	PRO	B	381	55.993	79.065	45.875	1.00	54.32
	2110	O	PRO	B	381	55.446	80.133	45.589	1.00	56.76
	2111	CB	PRO	B	381	57.664	79.375	47.740	1.00	60.70
	2112	CG	PRO	B	381	58.978	80.119	47.767	1.00	62.01
	2113	CD	PRO	B	381	58.905	80.945	46.526	1.00	59.24
	2114	N	VAL	B	382	55.356	77.899	45.866	1.00	55.74
	2115	CA	VAL	B	382	53.931	77.805	45.569	1.00	55.58
	2116	C	VAL	B	382	53.247	77.408	46.880	1.00	55.56
	2117	O	VAL	B	382	53.848	76.734	47.720	1.00	55.22
	2118	CB	VAL	B	382	53.620	76.726	44.493	1.00	55.39
	2119	CG1	VAL	B	382	54.404	77.008	43.222	1.00	55.94
	2120	CG2	VAL	B	382	53.936	75.339	45.025	1.00	53.06
	2121	N	ASN	B	383	52.000	77.827	47.055	1.00	54.38
	2122	CA	ASN	B	383	51.246	77.510	48.264	1.00	54.63
	2123	C	ASN	B	383	50.757	76.068	48.290	1.00	53.85
	2124	O	ASN	B	383	50.970	75.297	47.354	1.00	52.58
	2125	CB	ASN	B	383	50.034	78.429	48.382	1.00	59.07
	2126	CG	ASN	B	383	50.414	79.883	48.456	1.00	64.60
	2127	OD1	ASN	B	383	49.576	80.764	48.269	1.00	70.14
	2128	ND2	ASN	B	383	51.685	80.150	48.738	1.00	71.07
	2129	N	HIS	B	384	50.094	75.710	49.381	1.00	53.46
	2130	CA	HIS	B	384	49.543	74.371	49.526	1.00	52.22
	2131	C	HIS	B	384	48.298	74.274	48.640	1.00	49.10
	2132	O	HIS	B	384	47.495	75.200	48.585	1.00	45.53
	2133	CB	HIS	B	384	49.183	74.111	50.993	1.00	59.11
	2134	CG	HIS	B	384	50.377	73.924	51.878	1.00	62.16
	2135	ND1	HIS	B	384	51.243	72.862	51.739	1.00	69.15
	2136	CD2	HIS	B	384	50.855	74.669	52.903	1.00	70.28
	2137	CE1	HIS	B	384	52.206	72.960	52.639	1.00	75.01
	2138	NE2	HIS	B	384	51.995	74.047	53.358	1.00	74.58
	2139	N	SER	B	385	48.146	73.152	47.949	1.00	45.07
	2140	CA	SER	B	385	47.017	72.959	47.060	1.00	44.61
	2141	C	SER	B	385	45.973	71.983	47.604	1.00	44.58
	2142	O	SER	B	385	46.244	71.220	48.521	1.00	44.21

	2143	CB	SER	B	385	47.524	72.487	45.691	1.00	44.61
	2144	OG	SER	B	385	48.310	71.307	45.789	1.00	41.13
	2145	N	THR	B	386	44.773	72.025	47.035	1.00	44.32
	2146	CA	THR	B	386	43.684	71.150	47.446	1.00	44.35
	2147	C	THR	B	386	43.444	70.113	46.363	1.00	44.09
	2148	O	THR	B	386	43.274	70.451	45.189	1.00	44.06
	2149	CB	THR	B	386	42.374	71.936	47.680	1.00	45.20
	2150	OG1	THR	B	386	42.555	72.856	48.762	1.00	51.89
	2151	CG2	THR	B	386	41.232	70.984	48.036	1.00	47.20
	2152	N	ARG	B	387	43.424	68.851	46.774	1.00	44.39
	2153	CA	ARG	B	387	43.222	67.730	45.867	1.00	46.68
	2154	C	ARG	B	387	41.837	67.080	46.030	1.00	47.05
	2155	O	ARG	B	387	41.372	66.850	47.149	1.00	46.65
	2156	CB	ARG	B	387	44.316	66.694	46.121	1.00	48.13
	2157	CG	ARG	B	387	44.270	65.488	45.210	1.00	52.77
	2158	CD	ARG	B	387	45.106	64.353	45.780	1.00	56.60
	2159	NE	ARG	B	387	44.978	63.141	44.979	1.00	60.65
	2160	CZ	ARG	B	387	45.683	62.895	43.882	1.00	61.97
	2161	NH1	ARG	B	387	46.578	63.779	43.464	1.00	64.45
	2162	NH2	ARG	B	387	45.469	61.781	43.189	1.00	60.54
	2163	N	LYS	B	388	41.185	66.780	44.910	1.00	46.93
	2164	CA	LYS	B	388	39.870	66.143	44.933	1.00	47.51
	2165	C	LYS	B	388	39.823	64.970	43.957	1.00	48.33
	2166	O	LYS	B	388	40.199	65.107	42.794	1.00	46.08
	2167	CB	LYS	B	388	38.777	67.148	44.563	1.00	46.64
	2168	CG	LYS	B	388	38.691	68.326	45.497	1.00	52.75
	2169	CD	LYS	B	388	37.861	69.446	44.905	1.00	58.62
	2170	CE	LYS	B	388	38.062	70.737	45.682	1.00	62.49
	2171	NZ	LYS	B	388	37.396	71.881	44.999	1.00	67.33
	2172	N	GLU	B	389	39.364	63.820	44.449	1.00	50.07
	2173	CA	GLU	B	389	39.243	62.602	43.646	1.00	51.86
	2174	C	GLU	B	389	37.793	62.126	43.638	1.00	52.81
	2175	O	GLU	B	389	37.192	61.917	44.695	1.00	49.21
	2176	CB	GLU	B	389	40.126	61.494	44.223	1.00	54.67
	2177	CG	GLU	B	389	41.616	61.710	44.044	1.00	65.65
	2178	CD	GLU	B	389	42.441	60.608	44.688	1.00	72.66
	2179	OE1	GLU	B	389	42.151	59.418	44.429	1.00	75.92
	2180	OE2	GLU	B	389	43.380	60.931	45.450	1.00	75.78
	2181	N	GLU	B	390	37.229	61.948	42.449	1.00	56.06
	2182	CA	GLU	B	390	35.849	61.500	42.346	1.00	61.17
	2183	C	GLU	B	390	35.629	60.454	41.265	1.00	64.70
	2184	O	GLU	B	390	36.072	60.598	40.123	1.00	64.01
	2185	CB	GLU	B	390	34.927	62.692	42.107	1.00	64.35
	2186	CG	GLU	B	390	33.479	62.317	41.867	1.00	74.80
	2187	CD	GLU	B	390	32.548	63.509	41.979	1.00	85.97
	2188	OE1	GLU	B	390	32.822	64.547	41.336	1.00	92.60
	2189	OE2	GLU	B	390	31.541	63.403	42.712	1.00	92.18
	2190	N	LYS	B	391	34.921	59.396	41.639	1.00	68.18
	2191	CA	LYS	B	391	34.640	58.312	40.712	1.00	71.58
	2192	C	LYS	B	391	33.215	58.302	40.180	1.00	76.11
	2193	O	LYS	B	391	32.265	58.673	40.869	1.00	75.89
	2194	CB	LYS	B	391	34.946	56.973	41.372	1.00	67.28
	2195	N	GLN	B	392	33.092	57.876	38.932	1.00	81.85
	2196	CA	GLN	B	392	31.814	57.746	38.254	1.00	88.38
	2197	C	GLN	B	392	32.026	56.482	37.443	1.00	92.30
	2198	O	GLN	B	392	32.752	56.500	36.452	1.00	93.25
	2199	CB	GLN	B	392	31.555	58.938	37.323	1.00	85.87
	2200	CG	GLN	B	392	30.422	59.848	37.782	1.00	90.76
	2201	CD	GLN	B	392	30.027	60.873	36.731	1.00	93.39

	2202	OE1	GLN	B	392	29.687	60.524	35.598	1.00	92.93
	2203	NE2	GLN	B	392	30.062	62.147	37.107	1.00	93.97
	2204	N	ARG	B	393	31.426	55.379	37.880	1.00	96.24
	2205	CA	ARG	B	393	31.589	54.108	37.184	1.00	100.53
	2206	C	ARG	B	393	31.250	54.188	35.697	1.00	102.30
	2207	O	ARG	B	393	31.273	53.178	34.993	1.00	101.15
	2208	CB	ARG	B	393	30.747	53.021	37.855	1.00	106.99
	2209	CG	ARG	B	393	29.251	53.196	37.704	1.00	109.77
	2210	CD	ARG	B	393	28.521	52.107	38.464	1.00	115.73
	2211	NE	ARG	B	393	27.095	52.085	38.165	1.00	119.73
	2212	CZ	ARG	B	393	26.227	51.267	38.750	1.00	121.60
	2213	NH1	ARG	B	393	26.645	50.406	39.670	1.00	121.59
	2214	NH2	ARG	B	393	24.945	51.308	38.416	1.00	121.49
	2215	N	ASN	B	394	30.942	55.391	35.224	1.00	103.98
	2216	CA	ASN	B	394	30.630	55.595	33.819	1.00	106.60
	2217	C	ASN	B	394	31.918	55.325	33.049	1.00	106.89
	2218	O	ASN	B	394	31.950	54.516	32.122	1.00	108.55
	2219	CB	ASN	B	394	30.173	57.036	33.580	1.00	108.97
	2220	CG	ASN	B	394	29.709	57.274	32.153	1.00	112.83
	2221	OD1	ASN	B	394	29.459	58.410	31.752	1.00	114.53
	2222	ND2	ASN	B	394	29.584	56.198	31.381	1.00	114.40
	2223	N	GLY	B	395	32.984	56.007	33.452	1.00	105.53
	2224	CA	GLY	B	395	34.269	55.829	32.802	1.00	101.15
	2225	C	GLY	B	395	35.177	57.015	33.050	1.00	97.82
	2226	O	GLY	B	395	35.879	57.475	32.148	1.00	99.41
	2227	N	THR	B	396	35.177	57.516	34.278	1.00	94.50
	2228	CA	THR	B	396	36.011	58.663	34.578	1.00	89.02
	2229	C	THR	B	396	36.426	58.837	36.029	1.00	83.93
	2230	O	THR	B	396	35.600	59.123	36.896	1.00	83.27
	2231	CB	THR	B	396	35.322	59.975	34.130	1.00	92.03
	2232	OG1	THR	B	396	35.116	59.952	32.712	1.00	94.17
	2233	CG2	THR	B	396	36.179	61.186	34.504	1.00	95.48
	2234	N	LEU	B	397	37.718	58.658	36.279	1.00	79.69
	2235	CA	LEU	B	397	38.280	58.871	37.600	1.00	74.75
	2236	C	LEU	B	397	38.773	60.305	37.496	1.00	71.50
	2237	O	LEU	B	397	39.880	60.548	37.019	1.00	74.81
	2238	CB	LEU	B	397	39.480	57.960	37.860	1.00	75.72
	2239	CG	LEU	B	397	40.350	58.412	39.047	1.00	70.67
	2240	CD1	LEU	B	397	39.742	57.932	40.362	1.00	69.05
	2241	CD2	LEU	B	397	41.768	57.877	38.887	1.00	72.96
	2242	N	THR	B	398	37.941	61.252	37.905	1.00	67.61
	2243	CA	THR	B	398	38.314	62.655	37.848	1.00	61.30
	2244	C	THR	B	398	39.207	63.041	39.024	1.00	56.61
	2245	O	THR	B	398	38.974	62.640	40.166	1.00	54.95
	2246	CB	THR	B	398	37.070	63.556	37.852	1.00	61.75
	2247	OG1	THR	B	398	36.345	63.375	36.629	1.00	65.40
	2248	CG2	THR	B	398	37.471	65.016	37.992	1.00	63.39
	2249	N	VAL	B	399	40.241	63.817	38.729	1.00	51.84
	2250	CA	VAL	B	399	41.163	64.279	39.751	1.00	48.05
	2251	C	VAL	B	399	41.515	65.730	39.490	1.00	44.81
	2252	O	VAL	B	399	41.911	66.098	38.381	1.00	44.41
	2253	CB	VAL	B	399	42.466	63.468	39.751	1.00	49.35
	2254	CG1	VAL	B	399	43.409	64.010	40.805	1.00	49.43
	2255	CG2	VAL	B	399	42.168	62.006	40.010	1.00	53.10
	2256	N	THR	B	400	41.354	66.564	40.504	1.00	42.44
	2257	CA	THR	B	400	41.691	67.965	40.343	1.00	40.44
	2258	C	THR	B	400	42.532	68.449	41.498	1.00	38.07
	2259	O	THR	B	400	42.483	67.908	42.602	1.00	36.13
	2260	CB	THR	B	400	40.448	68.869	40.266	1.00	39.64
	2261	OG1	THR	B	400	39.845	68.962	41.561	1.00	43.72
	2262	CG2	THR	B	400	39.442	68.322	39.278	1.00	38.32
	2263	N	SER	B	401	43.335	69.460	41.216	1.00	36.90

	2264	CA	SER	B	401	44.168	70.069	42.224	1.00	35.46
	2265	C	SER	B	401	43.988	71.557	42.016	1.00	33.95
	2266	O	SER	B	401	44.153	72.062	40.908	1.00	34.80
	2267	CB	SER	B	401	45.638	69.694	42.040	1.00	36.91
	2268	OG	SER	B	401	46.417	70.301	43.060	1.00	40.84
	2269	N	THR	B	402	43.635	72.248	43.086	1.00	32.28
	2270	CA	THR	B	402	43.422	73.672	43.032	1.00	31.85
	2271	C	THR	B	402	44.508	74.355	43.836	1.00	31.76
	2272	O	THR	B	402	44.737	74.046	45.010	1.00	30.55
	2273	CB	THR	B	402	42.051	74.030	43.595	1.00	31.33
	2274	OG1	THR	B	402	41.058	73.316	42.862	1.00	32.83
	2275	CG2	THR	B	402	41.782	75.522	43.468	1.00	32.70
	2276	N	LEU	B	403	45.167	75.301	43.188	1.00	30.72
	2277	CA	LEU	B	403	46.257	76.018	43.800	1.00	30.33
	2278	C	LEU	B	403	45.927	77.485	44.003	1.00	29.66
	2279	O	LEU	B	403	45.608	78.185	43.048	1.00	28.06
	2280	CB	LEU	B	403	47.502	75.902	42.913	1.00	28.34
	2281	CG	LEU	B	403	48.769	76.632	43.381	1.00	32.10
	2282	CD1	LEU	B	403	49.425	75.823	44.503	1.00	31.94
	2283	CD2	LEU	B	403	49.756	76.790	42.224	1.00	30.42
	2284	N	PRO	B	404	45.983	77.962	45.259	1.00	31.48
	2285	CA	PRO	B	404	45.704	79.367	45.566	1.00	33.20
	2286	C	PRO	B	404	46.841	80.149	44.906	1.00	34.02
	2287	O	PRO	B	404	47.999	79.755	44.996	1.00	32.25
	2288	CB	PRO	B	404	45.788	79.417	47.090	1.00	33.28
	2289	CG	PRO	B	404	45.435	78.010	47.500	1.00	31.82
	2290	CD	PRO	B	404	46.186	77.187	46.497	1.00	31.26
	2291	N	VAL	B	405	46.503	81.238	44.235	1.00	34.94
	2292	CA	VAL	B	405	47.483	82.044	43.536	1.00	38.63
	2293	C	VAL	B	405	47.541	83.472	44.068	1.00	40.02
	2294	O	VAL	B	405	46.537	84.027	44.502	1.00	40.31
	2295	CB	VAL	B	405	47.143	82.052	42.018	1.00	42.09
	2296	CG1	VAL	B	405	47.110	83.472	41.468	1.00	43.95
	2297	CG2	VAL	B	405	48.144	81.195	41.273	1.00	41.76
	2298	N	GLY	B	406	48.728	84.064	44.039	1.00	42.35
	2299	CA	GLY	B	406	48.859	85.432	44.503	1.00	43.35
	2300	C	GLY	B	406	48.178	86.354	43.513	1.00	43.87
	2301	O	GLY	B	406	48.286	86.154	42.303	1.00	42.68
	2302	N	THR	B	407	47.466	87.352	44.023	1.00	44.40
	2303	CA	THR	B	407	46.760	88.306	43.177	1.00	47.37
	2304	C	THR	B	407	47.713	89.127	42.322	1.00	48.27
	2305	O	THR	B	407	47.549	89.208	41.107	1.00	48.77
	2306	CB	THR	B	407	45.922	89.288	44.022	1.00	48.44
	2307	OG1	THR	B	407	44.809	88.599	44.596	1.00	50.00
	2308	CG2	THR	B	407	45.413	90.436	43.162	1.00	53.23
	2309	N	ARG	B	408	48.697	89.746	42.970	1.00	48.10
	2310	CA	ARG	B	408	49.665	90.579	42.279	1.00	48.54
	2311	C	ARG	B	408	50.540	89.773	41.335	1.00	48.48
	2312	O	ARG	B	408	50.769	90.182	40.197	1.00	47.34
	2313	CB	ARG	B	408	50.530	91.325	43.290	1.00	50.16
	2314	N	ASP	B	409	51.033	88.634	41.806	1.00	48.72
	2315	CA	ASP	B	409	51.886	87.787	40.979	1.00	50.88
	2316	C	ASP	B	409	51.187	87.421	39.674	1.00	49.92
	2317	O	ASP	B	409	51.789	87.468	38.598	1.00	49.76
	2318	CB	ASP	B	409	52.260	86.512	41.738	1.00	56.18
	2319	CG	ASP	B	409	53.013	86.801	43.026	1.00	64.80
	2320	OD1	ASP	B	409	54.062	87.482	42.956	1.00	71.41
	2321	OD2	ASP	B	409	52.561	86.353	44.105	1.00	68.29
	2322	N	TRP	B	410	49.908	87.067	39.773	1.00	48.36
	2323	CA	TRP	B	410	49.142	86.686	38.597	1.00	46.32
	2324	C	TRP	B	410	48.953	87.864	37.653	1.00	46.21
	2325	O	TRP	B	410	49.111	87.731	36.440	1.00	44.64

	2326	CB	TRP	B	410	47.774	86.120	38.992	1.00	42.82
	2327	CG	TRP	B	410	47.001	85.710	37.796	1.00	39.31
	2328	CD1	TRP	B	410	46.104	86.467	37.103	1.00	37.29
	2329	CD2	TRP	B	410	47.181	84.507	37.043	1.00	35.49
	2330	NE1	TRP	B	410	45.726	85.819	35.957	1.00	39.24
	2331	CE2	TRP	B	410	46.372	84.613	35.895	1.00	32.76
	2332	CE3	TRP	B	410	47.956	83.351	37.228	1.00	32.07
	2333	CZ2	TRP	B	410	46.309	83.606	34.924	1.00	29.59
	2334	CZ3	TRP	B	410	47.896	82.352	36.269	1.00	33.68
	2335	CH2	TRP	B	410	47.073	82.489	35.125	1.00	30.56
	2336	N	ILE	B	411	48.611	89.016	38.212	1.00	48.11
	2337	CA	ILE	B	411	48.408	90.209	37.401	1.00	50.90
	2338	C	ILE	B	411	49.712	90.649	36.742	1.00	52.46
	2339	O	ILE	B	411	49.698	91.229	35.658	1.00	53.34
	2340	CB	ILE	B	411	47.845	91.366	38.246	1.00	51.58
	2341	CG1	ILE	B	411	46.456	90.987	38.770	1.00	52.81
	2342	CG2	ILE	B	411	47.772	92.634	37.415	1.00	51.95
	2343	CD1	ILE	B	411	45.823	92.034	39.669	1.00	59.38
	2344	N	GLU	B	412	50.837	90.348	37.385	1.00	53.21
	2345	CA	GLU	B	412	52.137	90.728	36.852	1.00	53.12
	2346	C	GLU	B	412	52.681	89.747	35.831	1.00	51.24
	2347	O	GLU	B	412	53.736	89.990	35.252	1.00	51.40
	2348	CB	GLU	B	412	53.152	90.909	37.981	1.00	59.71
	2349	CG	GLU	B	412	53.022	92.238	38.717	1.00	70.52
	2350	CD	GLU	B	412	54.060	92.399	39.810	1.00	78.58
	2351	OE1	GLU	B	412	55.262	92.198	39.527	1.00	83.44
	2352	OE2	GLU	B	412	53.676	92.732	40.950	1.00	82.10
	2353	N	GLY	B	413	51.982	88.634	35.623	1.00	48.47
	2354	CA	GLY	B	413	52.427	87.677	34.626	1.00	44.62
	2355	C	GLY	B	413	53.116	86.387	35.032	1.00	44.15
	2356	O	GLY	B	413	53.687	85.718	34.173	1.00	43.50
	2357	N	GLU	B	414	53.085	86.012	36.307	1.00	42.78
	2358	CA	GLU	B	414	53.722	84.757	36.694	1.00	40.78
	2359	C	GLU	B	414	53.105	83.652	35.851	1.00	39.97
	2360	O	GLU	B	414	51.955	83.758	35.410	1.00	37.43
	2361	CB	GLU	B	414	53.489	84.445	38.182	1.00	41.96
	2362	CG	GLU	B	414	54.034	83.081	38.659	1.00	44.09
	2363	CD	GLU	B	414	55.564	83.018	38.740	1.00	49.01
	2364	OE1	GLU	B	414	56.213	82.549	37.775	1.00	46.84
	2365	OE2	GLU	B	414	56.121	83.448	39.773	1.00	49.89
	2366	N	THR	B	415	53.879	82.599	35.615	1.00	39.56
	2367	CA	THR	B	415	53.403	81.464	34.847	1.00	40.76
	2368	C	THR	B	415	53.487	80.231	35.738	1.00	40.07
	2369	O	THR	B	415	54.533	79.960	36.323	1.00	42.10
	2370	CB	THR	B	415	54.238	81.273	33.556	1.00	44.69
	2371	OG1	THR	B	415	54.222	79.893	33.171	1.00	51.98
	2372	CG2	THR	B	415	55.652	81.744	33.758	1.00	50.00
	2373	N	TYR	B	416	52.380	79.500	35.860	1.00	37.57
	2374	CA	TYR	B	416	52.327	78.318	36.714	1.00	34.50
	2375	C	TYR	B	416	52.265	77.051	35.899	1.00	36.77
	2376	O	TYR	B	416	51.706	77.038	34.800	1.00	35.94
	2377	CB	TYR	B	416	51.116	78.379	37.634	1.00	34.15
	2378	CG	TYR	B	416	51.085	79.597	38.514	1.00	30.65
	2379	CD1	TYR	B	416	50.777	80.856	37.992	1.00	32.53
	2380	CD2	TYR	B	416	51.389	79.499	39.865	1.00	31.72
	2381	CE1	TYR	B	416	50.772	81.984	38.803	1.00	34.27
	2382	CE2	TYR	B	416	51.390	80.619	40.680	1.00	32.11
	2383	CZ	TYR	B	416	51.080	81.856	40.144	1.00	33.86
	2384	OH	TYR	B	416	51.082	82.964	40.961	1.00	41.22
	2385	N	GLN	B	417	52.829	75.976	36.441	1.00	37.58
	2386	CA	GLN	B	417	52.848	74.722	35.714	1.00	39.43
	2387	C	GLN	B	417	52.341	73.538	36.518	1.00	39.40

	2388	O	GLN	B	417	52.664	73.373	37.694	1.00	39.63
	2389	CB	GLN	B	417	54.269	74.421	35.211	1.00	41.37
	2390	CG	GLN	B	417	54.350	73.214	34.278	1.00	51.81
	2391	CD	GLN	B	417	55.773	72.856	33.886	1.00	61.69
	2392	OE1	GLN	B	417	56.555	72.371	34.710	1.00	67.15
	2393	NE2	GLN	B	417	56.219	73.096	32.621	1.00	63.64
	2394	N	CYS	B	418	51.543	72.712	35.864	1.00	39.29
	2395	CA	CYS	B	418	51.019	71.517	36.489	1.00	41.80
	2396	C	CYS	B	418	51.720	70.350	35.818	1.00	42.50
	2397	O	CYS	B	418	51.646	70.191	34.600	1.00	43.33
	2398	CB	CYS	B	418	49.501	71.392	36.275	1.00	41.95
	2399	SG	CYS	B	418	48.795	69.904	37.057	1.00	54.15
	2400	N	ARG	B	419	52.418	69.551	36.609	1.00	43.98
	2401	CA	ARG	B	419	53.103	68.375	36.093	1.00	47.51
	2402	C	ARG	B	419	52.277	67.172	36.542	1.00	48.11
	2403	O	ARG	B	419	52.219	66.859	37.730	1.00	47.85
	2404	CB	ARG	B	419	54.532	68.311	36.648	1.00	49.08
	2405	CG	ARG	B	419	55.203	66.958	36.514	1.00	54.11
	2406	CD	ARG	B	419	56.708	67.046	36.796	1.00	64.71
	2407	NE	ARG	B	419	57.325	65.732	36.963	1.00	64.09
	2408	CZ	ARG	B	419	57.437	65.107	38.132	1.00	70.31
	2409	NH1	ARG	B	419	56.981	65.681	39.239	1.00	68.32
	2410	NH2	ARG	B	419	57.992	63.901	38.195	1.00	71.53
	2411	N	VAL	B	420	51.610	66.524	35.592	1.00	51.04
	2412	CA	VAL	B	420	50.776	65.369	35.900	1.00	56.22
	2413	C	VAL	B	420	51.561	64.068	35.746	1.00	61.25
	2414	O	VAL	B	420	52.178	63.820	34.707	1.00	60.11
	2415	CB	VAL	B	420	49.536	65.305	34.985	1.00	54.44
	2416	CG1	VAL	B	420	48.678	64.106	35.371	1.00	52.69
	2417	CG2	VAL	B	420	48.732	66.597	35.095	1.00	55.45
	2418	N	THR	B	421	51.529	63.241	36.786	1.00	66.23
	2419	CA	THR	B	421	52.244	61.969	36.774	1.00	73.18
	2420	C	THR	B	421	51.334	60.766	36.970	1.00	76.87
	2421	O	THR	B	421	50.968	60.443	38.100	1.00	77.93
	2422	CB	THR	B	421	53.317	61.929	37.875	1.00	73.75
	2423	OG1	THR	B	421	54.272	62.972	37.649	1.00	77.71
	2424	CG2	THR	B	421	54.033	60.591	37.873	1.00	75.35
	2425	N	HIS	B	422	50.976	60.101	35.874	1.00	81.02
	2426	CA	HIS	B	422	50.117	58.922	35.949	1.00	86.07
	2427	C	HIS	B	422	51.004	57.686	35.822	1.00	89.67
	2428	O	HIS	B	422	51.920	57.653	35.002	1.00	90.00
	2429	CB	HIS	B	422	49.071	58.940	34.831	1.00	87.43
	2430	CG	HIS	B	422	47.892	58.052	35.092	1.00	90.73
	2431	ND1	HIS	B	422	47.076	58.203	36.191	1.00	93.83
	2432	CD2	HIS	B	422	47.396	57.000	34.396	1.00	91.89
	2433	CE1	HIS	B	422	46.127	57.282	36.164	1.00	94.70
	2434	NE2	HIS	B	422	46.300	56.540	35.085	1.00	93.25
	2435	N	PRO	B	423	50.729	56.646	36.626	1.00	92.64
	2436	CA	PRO	B	423	51.489	55.391	36.640	1.00	95.19
	2437	C	PRO	B	423	51.972	54.762	35.325	1.00	97.06
	2438	O	PRO	B	423	53.169	54.536	35.155	1.00	97.57
	2439	CB	PRO	B	423	50.576	54.445	37.433	1.00	95.56
	2440	CG	PRO	B	423	49.209	55.034	37.247	1.00	93.94
	2441	CD	PRO	B	423	49.488	56.495	37.404	1.00	93.12
	2442	N	HIS	B	424	51.058	54.495	34.399	1.00	98.71
	2443	CA	HIS	B	424	51.410	53.831	33.143	1.00	100.16
	2444	C	HIS	B	424	52.104	54.579	32.005	1.00	99.67
	2445	O	HIS	B	424	52.910	53.991	31.284	1.00	99.61
	2446	CB	HIS	B	424	50.165	53.149	32.578	1.00	102.42
	2447	CG	HIS	B	424	49.578	52.125	33.495	1.00	105.47
	2448	ND1	HIS	B	424	48.302	52.228	34.008	1.00	107.10
	2449	CD2	HIS	B	424	50.079	50.961	33.967	1.00	97.46

	2450	CE1	HIS	B	424	48.044	51.170	34.755	1.00	106.81
	2451	NE2	HIS	B	424	49.106	50.385	34.747	1.00	106.61
	2452	N	LEU	B	425	51.802	55.858	31.833	1.00	99.19
	2453	CA	LEU	B	425	52.384	56.628	30.737	1.00	99.01
	2454	C	LEU	B	425	53.886	56.908	30.816	1.00	98.36
	2455	O	LEU	B	425	54.440	57.121	31.896	1.00	98.39
	2456	CB	LEU	B	425	51.606	57.929	30.593	1.00	100.66
	2457	CG	LEU	B	425	50.105	57.631	30.633	1.00	101.95
	2458	CD1	LEU	B	425	49.315	58.917	30.531	1.00	102.59
	2459	CD2	LEU	B	425	49.744	56.677	29.502	1.00	103.85
	2460	N	PRO	B	426	54.562	56.915	29.652	1.00	97.57
	2461	CA	PRO	B	426	56.004	57.165	29.560	1.00	96.82
	2462	C	PRO	B	426	56.414	58.525	30.108	1.00	95.53
	2463	O	PRO	B	426	57.040	58.610	31.163	1.00	95.77
	2464	CB	PRO	B	426	56.282	57.030	28.063	1.00	97.13
	2465	CG	PRO	B	426	54.995	57.494	27.440	1.00	97.88
	2466	CD	PRO	B	426	53.969	56.798	28.307	1.00	97.70
	2467	N	ARG	B	427	56.064	59.585	29.387	1.00	94.16
	2468	CA	ARG	B	427	56.402	60.931	29.826	1.00	92.52
	2469	C	ARG	B	427	55.285	61.509	30.692	1.00	89.85
	2470	O	ARG	B	427	54.123	61.113	30.583	1.00	89.26
	2471	CB	ARG	B	427	56.652	61.851	28.622	1.00	97.34
	2472	CG	ARG	B	427	57.202	63.219	29.023	1.00	99.32
	2473	CD	ARG	B	427	57.407	64.172	27.847	1.00	105.99
	2474	NE	ARG	B	427	58.068	65.403	28.285	1.00	111.10
	2475	CZ	ARG	B	427	58.302	66.460	27.512	1.00	111.66
	2476	NH1	ARG	B	427	57.927	66.457	26.239	1.00	111.70
	2477	NH2	ARG	B	427	58.921	67.522	28.013	1.00	110.09
	2478	N	ALA	B	428	55.651	62.442	31.562	1.00	86.56
	2479	CA	ALA	B	428	54.690	63.087	32.439	1.00	82.70
	2480	C	ALA	B	428	53.998	64.211	31.677	1.00	80.03
	2481	O	ALA	B	428	54.619	64.889	30.861	1.00	80.29
	2482	CB	ALA	B	428	55.400	63.647	33.663	1.00	83.85
	2483	N	LEU	B	429	52.708	64.397	31.936	1.00	76.76
	2484	CA	LEU	B	429	51.949	65.456	31.285	1.00	72.72
	2485	C	LEU	B	429	52.311	66.780	31.936	1.00	69.67
	2486	O	LEU	B	429	52.472	66.858	33.153	1.00	68.64
	2487	CB	LEU	B	429	50.444	65.208	31.429	1.00	73.60
	2488	CG	LEU	B	429	49.753	64.431	30.307	1.00	73.35
	2489	CD1	LEU	B	429	48.320	64.102	30.696	1.00	72.09
	2490	CD2	LEU	B	429	49.787	65.267	29.035	1.00	76.40
	2491	N	MET	B	430	52.447	67.821	31.124	1.00	66.83
	2492	CA	MET	B	430	52.786	69.132	31.651	1.00	64.81
	2493	C	MET	B	430	51.922	70.216	31.026	1.00	61.41
	2494	O	MET	B	430	51.824	70.326	29.801	1.00	60.84
	2495	CB	MET	B	430	54.265	69.427	31.409	1.00	68.22
	2496	CG	MET	B	430	55.184	68.353	31.967	1.00	74.39
	2497	SD	MET	B	430	56.921	68.714	31.713	1.00	83.18
	2498	CE	MET	B	430	56.993	68.764	29.906	1.00	84.12
	2499	N	ARG	B	431	51.288	71.010	31.882	1.00	57.17
	2500	CA	ARG	B	431	50.428	72.094	31.426	1.00	54.04
	2501	C	ARG	B	431	50.848	73.366	32.137	1.00	50.58
	2502	O	ARG	B	431	51.233	73.330	33.304	1.00	50.46
	2503	CB	ARG	B	431	48.959	71.775	31.736	1.00	55.16
	2504	CG	ARG	B	431	48.413	70.564	30.991	1.00	59.24
	2505	CD	ARG	B	431	48.428	70.798	29.489	1.00	63.93
	2506	NE	ARG	B	431	48.014	69.617	28.737	1.00	70.30
	2507	CZ	ARG	B	431	48.043	69.530	27.411	1.00	76.24
	2508	NH1	ARG	B	431	48.469	70.559	26.683	1.00	77.83
	2509	NH2	ARG	B	431	47.648	68.415	26.811	1.00	77.12
	2510	N	SER	B	432	50.788	74.488	31.431	1.00	46.92
	2511	CA	SER	B	432	51.163	75.765	32.016	1.00	45.15

	2512	C	SER	B	432	50.118	76.816	31.702	1.00	42.49
	2513	O	SER	B	432	49.382	76.699	30.721	1.00	42.76
	2514	CB	SER	B	432	52.532	76.206	31.490	1.00	44.31
	2515	OG	SER	B	432	52.526	76.284	30.082	1.00	49.96
	2516	N	THR	B	433	50.060	77.851	32.530	1.00	40.28
	2517	CA	THR	B	433	49.078	78.909	32.337	1.00	39.71
	2518	C	THR	B	433	49.604	80.244	32.843	1.00	39.49
	2519	O	THR	B	433	50.414	80.285	33.766	1.00	40.22
	2520	CB	THR	B	433	47.761	78.577	33.078	1.00	38.07
	2521	OG1	THR	B	433	46.793	79.594	32.805	1.00	39.56
	2522	CG2	THR	B	433	47.991	78.512	34.582	1.00	36.99
	2523	N	THR	B	434	49.139	81.328	32.226	1.00	39.18
	2524	CA	THR	B	434	49.532	82.687	32.588	1.00	40.70
	2525	C	THR	B	434	48.414	83.635	32.166	1.00	40.23
	2526	O	THR	B	434	47.509	83.236	31.441	1.00	41.18
	2527	CB	THR	B	434	50.816	83.116	31.844	1.00	43.01
	2528	OG1	THR	B	434	50.548	83.238	30.439	1.00	47.85
	2529	CG2	THR	B	434	51.874	82.076	31.995	1.00	48.67
	2530	N	LYS	B	435	48.475	84.886	32.604	1.00	40.97
	2531	CA	LYS	B	435	47.450	85.833	32.211	1.00	45.73
	2532	C	LYS	B	435	47.579	85.999	30.702	1.00	48.93
	2533	O	LYS	B	435	48.670	85.890	30.158	1.00	48.49
	2534	CB	LYS	B	435	47.663	87.166	32.906	1.00	45.94
	2535	N	THR	B	436	46.467	86.235	30.018	1.00	52.01
	2536	CA	THR	B	436	46.520	86.429	28.574	1.00	54.88
	2537	C	THR	B	436	46.916	87.878	28.326	1.00	55.70
	2538	O	THR	B	436	46.454	88.777	29.023	1.00	55.21
	2539	CB	THR	B	436	45.146	86.162	27.909	1.00	56.24
	2540	OG1	THR	B	436	44.798	84.779	28.062	1.00	60.56
	2541	CG2	THR	B	436	45.188	86.510	26.423	1.00	57.04
	2542	N	SER	B	437	47.790	88.099	27.352	1.00	57.93
	2543	CA	SER	B	437	48.220	89.451	27.020	1.00	60.42
	2544	C	SER	B	437	47.361	89.917	25.851	1.00	60.49
	2545	O	SER	B	437	46.397	89.243	25.477	1.00	60.21
	2546	CB	SER	B	437	49.706	89.467	26.630	1.00	61.57
	2547	OG	SER	B	437	49.949	88.643	25.500	1.00	65.51
	2548	N	GLY	B	438	47.705	91.067	25.279	1.00	60.09
	2549	CA	GLY	B	438	46.934	91.578	24.161	1.00	58.42
	2550	C	GLY	B	438	45.970	92.663	24.589	1.00	57.80
	2551	O	GLY	B	438	45.853	92.952	25.778	1.00	56.51
	2552	N	PRO	B	439	45.267	93.291	23.633	1.00	57.81
	2553	CA	PRO	B	439	44.305	94.358	23.915	1.00	56.19
	2554	C	PRO	B	439	43.178	93.908	24.837	1.00	53.91
	2555	O	PRO	B	439	42.891	92.714	24.953	1.00	53.91
	2556	CB	PRO	B	439	43.794	94.735	22.524	1.00	57.79
	2557	CG	PRO	B	439	44.967	94.453	21.652	1.00	58.60
	2558	CD	PRO	B	439	45.427	93.115	22.179	1.00	60.65
	2559	N	ARG	B	440	42.545	94.878	25.488	1.00	51.09
	2560	CA	ARG	B	440	41.437	94.610	26.398	1.00	48.90
	2561	C	ARG	B	440	40.235	95.380	25.869	1.00	45.83
	2562	O	ARG	B	440	40.398	96.412	25.219	1.00	45.88
	2563	CB	ARG	B	440	41.764	95.099	27.811	1.00	49.95
	2564	CG	ARG	B	440	43.127	94.681	28.329	1.00	59.03
	2565	CD	ARG	B	440	43.227	93.194	28.652	1.00	65.31
	2566	NE	ARG	B	440	44.627	92.786	28.758	1.00	72.31
	2567	CZ	ARG	B	440	45.047	91.614	29.222	1.00	74.99
	2568	NH1	ARG	B	440	44.181	90.706	29.640	1.00	77.22
	2569	NH2	ARG	B	440	46.345	91.348	29.263	1.00	78.59
	2570	N	ALA	B	441	39.036	94.873	26.143	1.00	42.09
	2571	CA	ALA	B	441	37.800	95.521	25.713	1.00	39.26
	2572	C	ALA	B	441	36.706	95.124	26.687	1.00	38.22
	2573	O	ALA	B	441	36.566	93.951	27.024	1.00	38.95

	2574	CB	ALA	B	441	37.430	95.089	24.302	1.00	36.56
	2575	N	ALA	B	442	35.934	96.104	27.134	1.00	37.22
	2576	CA	ALA	B	442	34.871	95.861	28.089	1.00	37.60
	2577	C	ALA	B	442	33.721	95.050	27.510	1.00	38.65
	2578	O	ALA	B	442	33.497	95.047	26.302	1.00	40.22
	2579	CB	ALA	B	442	34.352	97.185	28.619	1.00	37.17
	2580	N	PRO	B	443	32.981	94.340	28.378	1.00	38.04
	2581	CA	PRO	B	443	31.835	93.511	27.996	1.00	36.79
	2582	C	PRO	B	443	30.581	94.376	27.857	1.00	38.14
	2583	O	PRO	B	443	30.426	95.364	28.579	1.00	37.39
	2584	CB	PRO	B	443	31.677	92.550	29.179	1.00	36.30
	2585	CG	PRO	B	443	32.968	92.654	29.941	1.00	36.35
	2586	CD	PRO	B	443	33.351	94.088	29.780	1.00	37.85
	2587	N	GLU	B	444	29.706	94.006	26.927	1.00	36.28
	2588	CA	GLU	B	444	28.437	94.699	26.729	1.00	35.57
	2589	C	GLU	B	444	27.429	93.659	27.212	1.00	33.87
	2590	O	GLU	B	444	27.495	92.490	26.809	1.00	33.43
	2591	CB	GLU	B	444	28.217	95.020	25.249	1.00	38.68
	2592	N	VAL	B	445	26.503	94.080	28.067	1.00	30.18
	2593	CA	VAL	B	445	25.530	93.168	28.650	1.00	28.24
	2594	C	VAL	B	445	24.077	93.464	28.289	1.00	28.44
	2595	O	VAL	B	445	23.625	94.600	28.379	1.00	26.78
	2596	CB	VAL	B	445	25.663	93.183	30.195	1.00	28.10
	2597	CG1	VAL	B	445	24.667	92.230	30.826	1.00	25.56
	2598	CG2	VAL	B	445	27.079	92.829	30.589	1.00	26.30
	2599	N	TYR	B	446	23.349	92.425	27.897	1.00	27.87
	2600	CA	TYR	B	446	21.949	92.581	27.549	1.00	27.91
	2601	C	TYR	B	446	21.140	91.407	28.076	1.00	27.06
	2602	O	TYR	B	446	21.293	90.274	27.620	1.00	27.96
	2603	CB	TYR	B	446	21.764	92.702	26.026	1.00	26.45
	2604	CG	TYR	B	446	20.311	92.851	25.653	1.00	26.59
	2605	CD1	TYR	B	446	19.543	93.886	26.195	1.00	28.48
	2606	CD2	TYR	B	446	19.686	91.941	24.795	1.00	29.02
	2607	CE1	TYR	B	446	18.183	94.011	25.896	1.00	33.24
	2608	CE2	TYR	B	446	18.326	92.057	24.484	1.00	31.33
	2609	CZ	TYR	B	446	17.585	93.094	25.041	1.00	36.01
	2610	OH	TYR	B	446	16.248	93.213	24.762	1.00	36.54
	2611	N	ALA	B	447	20.274	91.686	29.040	1.00	28.07
	2612	CA	ALA	B	447	19.450	90.651	29.661	1.00	27.67
	2613	C	ALA	B	447	18.021	90.785	29.168	1.00	29.19
	2614	O	ALA	B	447	17.564	91.898	28.927	1.00	31.10
	2615	CB	ALA	B	447	19.502	90.798	31.169	1.00	23.97
	2616	N	PHE	B	448	17.307	89.671	29.021	1.00	29.56
	2617	CA	PHE	B	448	15.943	89.751	28.522	1.00	32.50
	2618	C	PHE	B	448	15.117	88.525	28.854	1.00	33.67
	2619	O	PHE	B	448	15.650	87.488	29.228	1.00	35.26
	2620	CB	PHE	B	448	15.970	89.941	27.003	1.00	35.29
	2621	CG	PHE	B	448	16.523	88.751	26.262	1.00	37.04
	2622	CD1	PHE	B	448	15.691	87.688	25.905	1.00	36.66
	2623	CD2	PHE	B	448	17.886	88.666	25.973	1.00	34.95
	2624	CE1	PHE	B	448	16.218	86.551	25.276	1.00	40.91
	2625	CE2	PHE	B	448	18.422	87.534	25.347	1.00	35.99
	2626	CZ	PHE	B	448	17.586	86.477	24.997	1.00	35.15
	2627	N	ALA	B	449	13.804	88.648	28.704	1.00	35.81
	2628	CA	ALA	B	449	12.907	87.534	28.969	1.00	37.63
	2629	C	ALA	B	449	12.347	86.983	27.662	1.00	40.96
	2630	O	ALA	B	449	12.159	87.715	26.697	1.00	40.14
	2631	CB	ALA	B	449	11.769	87.977	29.870	1.00	33.60
	2632	N	THR	B	450	12.091	85.682	27.652	1.00	45.40
	2633	CA	THR	B	450	11.529	84.994	26.505	1.00	50.82
	2634	C	THR	B	450	10.003	85.085	26.602	1.00	53.78
	2635	O	THR	B	450	9.431	84.927	27.683	1.00	54.14

	2636	CB	THR	B	450	11.935	83.510	26.513	1.00	51.45
	2637	OG1	THR	B	450	13.358	83.408	26.650	1.00	54.12
	2638	CG2	THR	B	450	11.507	82.831	25.223	1.00	55.58
	2639	N	PRO	B	451	9.325	85.340	25.474	1.00	56.74
	2640	CA	PRO	B	451	7.863	85.443	25.477	1.00	59.05
	2641	C	PRO	B	451	7.209	84.173	26.020	1.00	61.00
	2642	O	PRO	B	451	7.520	83.065	25.579	1.00	59.71
	2643	CB	PRO	B	451	7.527	85.667	24.002	1.00	60.52
	2644	CG	PRO	B	451	8.749	86.338	23.460	1.00	61.14
	2645	CD	PRO	B	451	9.861	85.551	24.119	1.00	59.39
	2646	N	GLU	B	452	6.315	84.328	26.988	1.00	64.30
	2647	CA	GLU	B	452	5.625	83.172	27.542	1.00	69.17
	2648	C	GLU	B	452	4.137	83.348	27.258	1.00	72.61
	2649	O	GLU	B	452	3.394	83.933	28.043	1.00	73.59
	2650	CB	GLU	B	452	5.838	83.040	29.046	1.00	65.66
	2651	CG	GLU	B	452	6.034	81.585	29.523	1.00	61.46
	2652	CD	GLU	B	452	7.283	80.883	28.967	1.00	60.52
	2653	OE1	GLU	B	452	8.336	81.547	28.849	1.00	63.47
	2654	OE2	GLU	B	452	7.227	79.666	28.667	1.00	53.34
	2655	N	TRP	B	453	3.731	82.837	26.103	1.00	76.75
	2656	CA	TRP	B	453	2.358	82.907	25.619	1.00	81.00
	2657	C	TRP	B	453	1.573	81.714	26.187	1.00	82.30
	2658	O	TRP	B	453	1.890	80.562	25.885	1.00	82.08
	2659	CB	TRP	B	453	2.409	82.863	24.090	1.00	85.65
	2660	CG	TRP	B	453	1.233	83.418	23.366	1.00	89.76
	2661	CD1	TRP	B	453	0.679	84.661	23.512	1.00	92.34
	2662	CD2	TRP	B	453	0.517	82.781	22.305	1.00	94.15
	2663	NE1	TRP	B	453	-0.334	84.836	22.598	1.00	94.99
	2664	CE2	TRP	B	453	-0.455	83.696	21.845	1.00	95.56
	2665	CE3	TRP	B	453	0.605	81.521	21.693	1.00	95.36
	2666	CZ2	TRP	B	453	-1.335	83.392	20.800	1.00	97.14
	2667	CZ3	TRP	B	453	-0.269	81.220	20.655	1.00	95.61
	2668	CH2	TRP	B	453	-1.226	82.153	20.220	1.00	97.12
	2669	N	PRO	B	454	0.542	81.981	27.020	1.00	84.10
	2670	CA	PRO	B	454	-0.331	80.994	27.678	1.00	87.24
	2671	C	PRO	B	454	-0.716	79.708	26.938	1.00	90.52
	2672	O	PRO	B	454	-0.378	79.512	25.767	1.00	89.75
	2673	CB	PRO	B	454	-1.550	81.825	28.112	1.00	84.91
	2674	CG	PRO	B	454	-1.417	83.125	27.360	1.00	83.62
	2675	CD	PRO	B	454	0.063	83.341	27.307	1.00	84.60
	2676	N	GLY	B	455	-1.455	78.849	27.636	1.00	91.72
	2677	CA	GLY	B	455	-1.813	77.552	27.088	1.00	94.13
	2678	C	GLY	B	455	-0.532	76.870	27.499	1.00	96.28
	2679	O	GLY	B	455	0.475	76.987	26.799	1.00	97.74
	2680	N	SER	B	456	-0.542	76.158	28.622	1.00	99.11
	2681	CA	SER	B	456	0.731	75.626	29.077	1.00	96.15
	2682	C	SER	B	456	1.135	74.193	29.424	1.00	91.50
	2683	O	SER	B	456	0.316	73.308	29.767	1.00	88.52
	2684	CB	SER	B	456	1.222	76.508	30.221	1.00	95.05
	2685	OG	SER	B	456	0.225	76.690	31.216	1.00	110.76
	2686	N	ARG	B	457	2.464	74.059	29.348	1.00	87.73
	2687	CA	ARG	B	457	3.349	72.936	29.580	1.00	87.81
	2688	C	ARG	B	457	4.497	73.922	29.453	1.00	86.30
	2689	O	ARG	B	457	4.602	74.574	28.403	1.00	90.57
	2690	CB	ARG	B	457	3.339	71.966	28.425	1.00	94.67
	2691	N	ASP	B	458	5.341	74.088	30.473	1.00	87.32
	2692	CA	ASP	B	458	6.314	75.159	30.320	1.00	80.43
	2693	C	ASP	B	458	7.637	75.178	31.020	1.00	72.83

	2694	O	ASP	B	458	8.163	74.190	31.501	1.00	73.96
	2695	CB	ASP	B	458	5.615	76.450	30.715	1.00	83.19
	2696	CG	ASP	B	458	5.300	76.498	32.210	1.00	85.09
5	2697	OD1	ASP	B	458	4.694	75.535	32.722	1.00	91.25
	2698	OD2	ASP	B	458	5.661	77.492	32.883	1.00	90.84
	2699	N	LYS	B	459	8.149	76.404	31.024	1.00	66.05
	2700	CA	LYS	B	459	9.389	76.818	31.663	1.00	61.75
	2701	C	LYS	B	459	9.617	78.232	31.214	1.00	56.14
10	2702	O	LYS	B	459	9.952	78.456	30.054	1.00	56.54
	2703	CB	LYS	B	459	10.569	75.959	31.211	1.00	68.18
	2704	CG	LYS	B	459	10.796	74.799	32.131	1.00	71.85
	2705	CD	LYS	B	459	10.737	75.194	33.601	1.00	73.79
	2706	CE	LYS	B	459	10.761	73.945	34.474	1.00	76.14
15	2707	NZ	LYS	B	459	10.925	74.259	35.931	1.00	79.35
	2708	N	ARG	B	460	9.406	79.194	32.099	1.00	52.32
	2709	CA	ARG	B	460	9.649	80.565	31.723	1.00	47.59
	2710	C	ARG	B	460	11.164	80.740	31.810	1.00	43.34
	2711	O	ARG	B	460	11.839	80.123	32.638	1.00	40.40
20	2712	CB	ARG	B	460	8.874	81.496	32.644	1.00	49.27
	2713	CG	ARG	B	460	7.384	81.325	32.429	1.00	56.23
	2714	CD	ARG	B	460	6.594	81.941	33.568	1.00	63.20
	2715	NE	ARG	B	460	5.174	81.603	33.504	1.00	68.02
	2716	CZ	ARG	B	460	4.645	80.455	33.920	1.00	70.46
25	2717	NH1	ARG	B	460	5.415	79.506	34.444	1.00	72.23
	2718	NH2	ARG	B	460	3.336	80.264	33.815	1.00	73.53
	2719	N	THR	B	461	11.690	81.538	30.902	1.00	39.19
	2720	CA	THR	B	461	13.126	81.721	30.822	1.00	36.81
	2721	C	THR	B	461	13.596	83.153	30.699	1.00	34.03
30	2722	O	THR	B	461	12.993	83.969	29.990	1.00	33.96
	2723	CB	THR	B	461	13.710	80.997	29.588	1.00	39.13
	2724	OG1	THR	B	461	13.243	79.643	29.543	1.00	46.04
	2725	CG2	THR	B	461	15.220	80.970	29.679	1.00	45.48
	2726	N	LEU	B	462	14.696	83.443	31.386	1.00	29.84
35	2727	CA	LEU	B	462	15.333	84.747	31.312	1.00	28.03
	2728	C	LEU	B	462	16.674	84.395	30.690	1.00	27.33
	2729	O	LEU	B	462	17.186	83.293	30.893	1.00	24.47
	2730	CB	LEU	B	462	15.526	85.377	32.697	1.00	25.97
	2731	CG	LEU	B	462	14.238	85.712	33.465	1.00	33.39
40	2732	CD1	LEU	B	462	14.593	86.428	34.781	1.00	32.36
	2733	CD2	LEU	B	462	13.337	86.586	32.617	1.00	30.72
	2734	N	ALA	B	463	17.241	85.314	29.922	1.00	25.83
	2735	CA	ALA	B	463	18.489	85.023	29.264	1.00	25.65
	2736	C	ALA	B	463	19.321	86.270	29.143	1.00	26.32
45	2737	O	ALA	B	463	18.810	87.386	29.254	1.00	27.53
	2738	CB	ALA	B	463	18.219	84.421	27.888	1.00	28.15
	2739	N	CYS	B	464	20.608	86.082	28.905	1.00	21.23
	2740	CA	CYS	B	464	21.507	87.212	28.824	1.00	24.77
	2741	C	CYS	B	464	22.584	87.001	27.786	1.00	22.14
50	2742	O	CYS	B	464	23.169	85.917	27.698	1.00	24.66
	2743	CB	CYS	B	464	22.171	87.407	30.186	1.00	22.04
	2744	SG	CYS	B	464	23.302	88.810	30.380	1.00	34.06
	2745	N	LEU	B	465	22.859	88.052	27.025	1.00	22.44
	2746	CA	LEU	B	465	23.903	88.002	26.011	1.00	23.11
55	2747	C	LEU	B	465	24.985	88.956	26.459	1.00	22.43
	2748	O	LEU	B	465	24.702	90.117	26.748	1.00	23.73
	2749	CB	LEU	B	465	23.370	88.445	24.639	1.00	22.99
	2750	CG	LEU	B	465	24.423	88.790	23.562	1.00	19.04
	2751	CD1	LEU	B	465	25.269	87.565	23.234	1.00	21.72
5	2752	CD2	LEU	B	465	23.716	89.253	22.282	1.00	28.23
	2753	N	ILE	B	466	26.220	88.475	26.519	1.00	22.56
	2754	CA	ILE	B	466	27.332	89.323	26.931	1.00	22.11
	2755	C	ILE	B	466	28.344	89.298	25.803	1.00	24.25

	2756	O	ILE	B	466	28.785	88.225	25.394	1.00	24.93
	2757	CB	ILE	B	466	27.946	88.819	28.239	1.00	22.15
	2758	CG1	ILE	B	466	26.850	88.751	29.314	1.00	23.07
	2759	CG2	ILE	B	466	29.075	89.778	28.684	1.00	25.24
	2760	CD1	ILE	B	466	27.282	88.091	30.604	1.00	33.12
	2761	N	GLN	B	467	28.737	90.468	25.307	1.00	24.63
	2762	CA	GLN	B	467	29.630	90.480	24.149	1.00	28.64
	2763	C	GLN	B	467	30.637	91.618	24.028	1.00	31.08
	2764	O	GLN	B	467	30.685	92.529	24.865	1.00	31.00
	2765	CB	GLN	B	467	28.770	90.428	22.872	1.00	25.58
	2766	CG	GLN	B	467	27.873	91.657	22.696	1.00	25.53
	2767	CD	GLN	B	467	26.907	91.556	21.501	1.00	30.72
	2768	OE1	GLN	B	467	27.144	90.810	20.551	1.00	29.76
	2769	NE2	GLN	B	467	25.821	92.327	21.550	1.00	32.18
	2770	N	ASN	B	468	31.453	91.517	22.977	1.00	33.71
	2771	CA	ASN	B	468	32.494	92.486	22.641	1.00	36.96
	2772	C	ASN	B	468	33.601	92.607	23.677	1.00	38.20
	2773	O	ASN	B	468	34.208	93.669	23.812	1.00	38.39
	2774	CB	ASN	B	468	31.881	93.869	22.424	1.00	41.06
	2775	CG	ASN	B	468	30.763	93.852	21.414	1.00	46.41
	2776	OD1	ASN	B	468	30.879	93.228	20.359	1.00	50.82
	2777	ND2	ASN	B	468	29.672	94.548	21.724	1.00	53.31
	2778	N	PHE	B	469	33.868	91.535	24.415	1.00	35.74
	2779	CA	PHE	B	469	34.910	91.597	25.423	1.00	33.87
	2780	C	PHE	B	469	36.147	90.796	25.044	1.00	33.63
	2781	O	PHE	B	469	36.087	89.873	24.240	1.00	34.78
	2782	CB	PHE	B	469	34.372	91.105	26.778	1.00	29.12
	2783	CG	PHE	B	469	33.909	89.674	26.766	1.00	26.27
	2784	CD1	PHE	B	469	34.808	88.641	26.967	1.00	22.45
	2785	CD2	PHE	B	469	32.566	89.362	26.561	1.00	22.06
	2786	CE1	PHE	B	469	34.386	87.315	26.974	1.00	23.84
	2787	CE2	PHE	B	469	32.135	88.036	26.564	1.00	28.02
	2788	CZ	PHE	B	469	33.051	87.007	26.773	1.00	23.33
	2789	N	MET	B	470	37.273	91.169	25.634	1.00	35.64
	2790	CA	MET	B	470	38.535	90.480	25.413	1.00	37.62
	2791	C	MET	B	470	39.496	90.916	26.504	1.00	36.36
	2792	O	MET	B	470	39.478	92.071	26.923	1.00	36.33
	2793	CB	MET	B	470	39.105	90.796	24.024	1.00	42.61
	2794	CG	MET	B	470	39.421	92.246	23.750	1.00	50.60
	2795	SD	MET	B	470	39.856	92.459	21.987	1.00	66.08
	2796	CE	MET	B	470	41.544	91.820	21.966	1.00	66.35
	2797	N	PRO	B	471	40.317	89.987	27.021	1.00	34.63
	2798	CA	PRO	B	471	40.431	88.561	26.682	1.00	32.61
	2799	C	PRO	B	471	39.147	87.782	26.957	1.00	31.92
	2800	O	PRO	B	471	38.164	88.356	27.415	1.00	29.59
	2801	CB	PRO	B	471	41.585	88.080	27.562	1.00	33.95
	2802	CG	PRO	B	471	42.373	89.323	27.805	1.00	37.90
	2803	CD	PRO	B	471	41.309	90.354	28.042	1.00	34.78
	2804	N	GLU	B	472	39.187	86.472	26.714	1.00	32.28
	2805	CA	GLU	B	472	38.020	85.599	26.866	1.00	36.49
	2806	C	GLU	B	472	37.557	85.220	28.270	1.00	35.52
	2807	O	GLU	B	472	36.438	84.730	28.417	1.00	34.87
	2808	CB	GLU	B	472	38.223	84.298	26.085	1.00	41.97
	2809	CG	GLU	B	472	39.294	83.387	26.677	1.00	54.78
	2810	CD	GLU	B	472	39.456	82.073	25.916	1.00	62.41
	2811	OE1	GLU	B	472	39.021	81.997	24.744	1.00	67.26
	2812	OE2	GLU	B	472	40.034	81.119	26.487	1.00	64.96
	2813	N	ASP	B	473	38.379	85.439	29.295	1.00	34.38
	2814	CA	ASP	B	473	37.971	85.057	30.648	1.00	31.83
	2815	C	ASP	B	473	36.914	85.998	31.214	1.00	31.24
	2816	O	ASP	B	473	37.072	87.220	31.199	1.00	31.80
	2817	CB	ASP	B	473	39.180	84.979	31.584	1.00	34.73

	2818	CG	ASP	B	473	40.147	83.854	31.196	1.00	40.83
	2819	OD1	ASP	B	473	39.676	82.759	30.804	1.00	44.18
	2820	OD2	ASP	B	473	41.378	84.061	31.290	1.00	40.17
	2821	N	ILE	B	474	35.826	85.416	31.702	1.00	26.96
	2822	CA	ILE	B	474	34.744	86.207	32.246	1.00	25.39
	2823	C	ILE	B	474	33.885	85.375	33.208	1.00	24.74
	2824	O	ILE	B	474	33.776	84.164	33.069	1.00	25.20
	2825	CB	ILE	B	474	33.862	86.758	31.092	1.00	23.81
	2826	CG1	ILE	B	474	32.925	87.852	31.598	1.00	22.23
	2827	CG2	ILE	B	474	33.062	85.626	30.453	1.00	27.10
	2828	CD1	ILE	B	474	32.144	88.536	30.450	1.00	25.30
	2829	N	SER	B	475	33.312	86.030	34.209	1.00	23.27
	2830	CA	SER	B	475	32.430	85.348	35.148	1.00	22.17
	2831	C	SER	B	475	31.066	85.991	34.952	1.00	21.71
	2832	O	SER	B	475	30.951	87.207	34.876	1.00	20.84
	2833	CB	SER	B	475	32.879	85.551	36.593	1.00	20.43
	2834	OG	SER	B	475	34.164	85.011	36.806	1.00	30.00
	2835	N	VAL	B	476	30.042	85.158	34.887	1.00	21.76
	2836	CA	VAL	B	476	28.694	85.620	34.675	1.00	21.72
	2837	C	VAL	B	476	27.875	85.165	35.851	1.00	23.56
	2838	O	VAL	B	476	28.036	84.045	36.320	1.00	25.95
	2839	CB	VAL	B	476	28.087	84.994	33.385	1.00	21.56
	2840	CG1	VAL	B	476	26.625	85.443	33.222	1.00	18.70
	2841	CG2	VAL	B	476	28.915	85.403	32.166	1.00	20.99
	2842	N	GLN	B	477	26.994	86.026	36.336	1.00	25.16
	2843	CA	GLN	B	477	26.172	85.635	37.460	1.00	26.65
	2844	C	GLN	B	477	24.833	86.337	37.438	1.00	26.62
	2845	O	GLN	B	477	24.709	87.440	36.925	1.00	26.40
	2846	CB	GLN	B	477	26.917	85.899	38.775	1.00	31.51
	2847	CG	GLN	B	477	27.348	87.311	39.011	1.00	44.27
	2848	CD	GLN	B	477	28.505	87.412	40.016	1.00	47.76
	2849	OE1	GLN	B	477	28.814	88.496	40.502	1.00	50.57
	2850	NE2	GLN	B	477	29.151	86.283	40.313	1.00	47.32
	2851	N	TRP	B	478	23.820	85.659	37.954	1.00	27.41
	2852	CA	TRP	B	478	22.488	86.225	38.026	1.00	28.36
	2853	C	TRP	B	478	22.192	86.656	39.465	1.00	30.10
	2854	O	TRP	B	478	22.660	86.033	40.428	1.00	25.31
	2855	CB	TRP	B	478	21.461	85.196	37.567	1.00	28.76
	2856	CG	TRP	B	478	21.502	84.951	36.087	1.00	34.11
	2857	CD1	TRP	B	478	22.313	84.078	35.415	1.00	31.25
	2858	CD2	TRP	B	478	20.722	85.620	35.094	1.00	31.01
	2859	NE1	TRP	B	478	22.085	84.164	34.069	1.00	27.71
	2860	CE2	TRP	B	478	21.113	85.104	33.841	1.00	31.95
	2861	CE3	TRP	B	478	19.729	86.607	35.140	1.00	34.16
	2862	CZ2	TRP	B	478	20.542	85.545	32.637	1.00	25.26
	2863	CZ3	TRP	B	478	19.161	87.044	33.947	1.00	31.64
	2864	CH2	TRP	B	478	19.571	86.511	32.713	1.00	28.89
	2865	N	LEU	B	479	21.418	87.723	39.602	1.00	32.48
	2866	CA	LEU	B	479	21.049	88.245	40.913	1.00	37.36
	2867	C	LEU	B	479	19.584	88.657	40.960	1.00	40.42
	2868	O	LEU	B	479	19.040	89.152	39.977	1.00	40.14
	2869	CB	LEU	B	479	21.878	89.478	41.252	1.00	39.83
	2870	CG	LEU	B	479	23.346	89.556	40.842	1.00	44.57
	2871	CD1	LEU	B	479	23.890	90.887	41.290	1.00	52.98
	2872	CD2	LEU	B	479	24.130	88.439	41.466	1.00	50.71
	2873	N	HIS	B	480	18.947	88.448	42.102	1.00	43.05
	2874	CA	HIS	B	480	17.572	88.877	42.276	1.00	49.20
	2875	C	HIS	B	480	17.746	90.136	43.116	1.00	52.73
	2876	O	HIS	B	480	17.705	90.091	44.347	1.00	52.90
	2877	CB	HIS	B	480	16.754	87.844	43.043	1.00	52.25
	2878	CG	HIS	B	480	15.341	88.270	43.286	1.00	57.22
	2879	ND1	HIS	B	480	14.337	88.075	42.364	1.00	61.37

	2880	CD2	HIS	B	480	14.778	88.942	44.319	1.00	59.16
	2881	CE1	HIS	B	480	13.216	88.607	42.815	1.00	59.88
	2882	NE2	HIS	B	480	13.456	89.140	44.000	1.00	66.11
	2883	N	ASN	B	481	17.971	91.253	42.430	1.00	56.65
	2884	CA	ASN	B	481	18.206	92.543	43.070	1.00	59.93
	2885	C	ASN	B	481	19.660	92.591	43.519	1.00	59.65
	2886	O	ASN	B	481	20.571	92.569	42.695	1.00	61.04
	2887	CB	ASN	B	481	17.288	92.751	44.282	1.00	64.65
	2888	CG	ASN	B	481	15.852	93.022	43.890	1.00	72.38
	2889	OD1	ASN	B	481	15.563	93.964	43.147	1.00	74.96
	2890	ND2	ASN	B	481	14.938	92.199	44.393	1.00	75.60
	2891	N	GLU	B	482	19.872	92.625	44.827	1.00	58.97
	2892	CA	GLU	B	482	21.213	92.697	45.396	1.00	58.55
	2893	C	GLU	B	482	21.815	91.346	45.782	1.00	55.30
	2894	O	GLU	B	482	23.013	91.253	46.044	1.00	57.27
	2895	CB	GLU	B	482	21.176	93.607	46.627	1.00	65.42
	2896	CG	GLU	B	482	19.760	93.813	47.172	1.00	73.94
	2897	CD	GLU	B	482	19.735	94.473	48.532	1.00	80.29
	2898	OE1	GLU	B	482	20.168	93.830	49.513	1.00	86.31
	2899	OE2	GLU	B	482	19.284	95.633	48.620	1.00	82.73
	2900	N	VAL	B	483	20.997	90.301	45.814	1.00	50.25
	2901	CA	VAL	B	483	21.487	88.988	46.211	1.00	45.78
	2902	C	VAL	B	483	21.733	88.025	45.052	1.00	43.04
	2903	O	VAL	B	483	20.880	87.834	44.198	1.00	41.34
	2904	CB	VAL	B	483	20.527	88.339	47.233	1.00	43.76
	2905	CG1	VAL	B	483	19.129	88.283	46.668	1.00	46.25
	2906	CG2	VAL	B	483	21.011	86.946	47.594	1.00	41.37
	2907	N	GLN	B	484	22.912	87.412	45.050	1.00	42.30
	2908	CA	GLN	B	484	23.300	86.474	44.005	1.00	43.21
	2909	C	GLN	B	484	22.658	85.091	44.141	1.00	42.48
	2910	O	GLN	B	484	22.538	84.545	45.244	1.00	41.64
	2911	CB	GLN	B	484	24.826	86.331	43.971	1.00	45.96
	2912	CG	GLN	B	484	25.324	85.269	42.999	1.00	54.43
	2913	CD	GLN	B	484	26.840	85.173	42.941	1.00	59.02
	2914	OE1	GLN	B	484	27.391	84.200	42.423	1.00	59.71
	2915	NE2	GLN	B	484	27.522	86.190	43.464	1.00	61.46
	2916	N	LEU	B	485	22.239	84.539	43.006	1.00	38.99
	2917	CA	LEU	B	485	21.618	83.218	42.953	1.00	39.17
	2918	C	LEU	B	485	22.700	82.142	43.853	1.00	40.35
	2919	O	LEU	B	485	23.822	82.417	42.430	1.00	37.39
	2920	CB	LEU	B	485	20.705	83.107	41.725	1.00	37.16
	2921	CG	LEU	B	485	19.579	84.140	41.602	1.00	39.66
	2922	CD1	LEU	B	485	18.836	83.930	40.293	1.00	39.30
	2923	CD2	LEU	B	485	18.644	84.020	42.795	1.00	40.56
	2924	N	PRO	B	486	22.373	80.900	43.242	1.00	42.55
	2925	CA	PRO	B	486	23.366	79.828	43.158	1.00	46.30
	2926	C	PRO	B	486	23.750	79.660	41.688	1.00	49.32
	2927	O	PRO	B	486	22.916	79.852	40.806	1.00	48.81
	2928	CB	PRO	B	486	22.606	78.609	43.675	1.00	45.64
	2929	CG	PRO	B	486	21.532	79.187	44.528	1.00	45.29
	2930	CD	PRO	B	486	21.095	80.394	43.769	1.00	40.65
	2931	N	ASP	B	487	24.997	79.290	41.429	1.00	53.39
	2932	CA	ASP	B	487	25.465	79.093	40.062	1.00	57.75
	2933	C	ASP	B	487	24.660	77.997	39.350	1.00	57.25
	2934	O	ASP	B	487	24.305	78.176	38.213	1.00	57.75
	2935	CB	ASP	B	487	26.944	78.708	40.077	1.00	67.82
	2936	CG	ASP	B	487	27.577	78.779	38.703	1.00	76.17
	2937	OD1	ASP	B	487	26.945	78.309	37.734	1.00	84.77
	2938	OD2	ASP	B	487	28.711	79.297	38.592	1.00	86.94
	2939	N	ALA	B	488	24.478	76.873	40.035	1.00	54.64
	2940	CA	ALA	B	488	23.752	75.729	39.493	1.00	53.45
	2941	C	ALA	B	488	22.421	76.069	38.837	1.00	52.74

	2942	O	ALA	B	488	21.843	75.241	38.134	1.00	53.06
	2943	CB	ALA	B	488	23.530	74.708	40.585	1.00	53.75
	2944	N	ARG	B	489	21.938	77.287	39.056	1.00	50.96
	2945	CA	ARG	B	489	20.660	77.704	38.491	1.00	47.84
	2946	C	ARG	B	489	20.705	78.164	37.036	1.00	45.10
	2947	O	ARG	B	489	19.681	78.158	36.363	1.00	43.37
	2948	CB	ARG	B	489	20.046	78.808	39.354	1.00	48.99
	2949	CG	ARG	B	489	19.232	78.294	40.524	1.00	50.01
	2950	CD	ARG	B	489	17.761	78.427	40.227	1.00	50.36
	2951	NE	ARG	B	489	17.187	79.581	40.905	1.00	56.65
	2952	CZ	ARG	B	489	16.048	80.166	40.557	1.00	58.23
	2953	NH1	ARG	B	489	15.352	79.714	39.522	1.00	61.07
	2954	NH2	ARG	B	489	15.594	81.193	41.260	1.00	59.63
	2955	N	HIS	B	490	21.872	78.573	36.551	1.00	42.41
	2956	CA	HIS	B	490	21.965	79.024	35.166	1.00	41.63
	2957	C	HIS	B	490	22.952	78.210	34.334	1.00	39.71
	2958	O	HIS	B	490	23.768	77.471	34.865	1.00	41.30
	2959	CB	HIS	B	490	22.348	80.508	35.100	1.00	42.40
	2960	CG	HIS	B	490	23.720	80.807	35.614	1.00	43.27
	2961	ND1	HIS	B	490	23.966	81.177	36.919	1.00	42.27
	2962	CD2	HIS	B	490	24.926	80.779	34.999	1.00	44.41
	2963	CE1	HIS	B	490	25.262	81.364	37.086	1.00	39.88
	2964	NE2	HIS	B	490	25.868	81.130	35.934	1.00	45.37
	2965	N	SER	B	491	22.858	78.355	33.020	1.00	37.20
	2966	CA	SER	B	491	23.734	77.654	32.095	1.00	36.36
	2967	C	SER	B	491	24.401	78.685	31.173	1.00	33.06
	2968	O	SER	B	491	23.721	79.428	30.461	1.00	33.77
	2969	CB	SER	B	491	22.910	76.651	31.288	1.00	35.42
	2970	OG	SER	B	491	23.694	76.053	30.282	1.00	43.65
	2971	N	THR	B	492	25.728	78.722	31.188	1.00	29.90
	2972	CA	THR	B	492	26.495	79.673	30.383	1.00	29.91
	2973	C	THR	B	492	27.322	78.977	29.287	1.00	29.20
	2974	O	THR	B	492	27.996	77.991	29.552	1.00	30.85
	2975	CB	THR	B	492	27.447	80.506	31.298	1.00	29.85
	2976	OG1	THR	B	492	26.670	81.197	32.281	1.00	35.86
	2977	CG2	THR	B	492	28.234	81.541	30.498	1.00	28.05
	2978	N	THR	B	493	27.281	79.505	28.065	1.00	29.49
	2979	CA	THR	B	493	28.032	78.913	26.957	1.00	30.19
	2980	C	THR	B	493	29.501	79.295	27.056	1.00	32.39
	2981	O	THR	B	493	29.863	80.210	27.786	1.00	30.70
	2982	CB	THR	B	493	27.502	79.378	25.568	1.00	27.82
	2983	OG1	THR	B	493	27.592	80.806	25.460	1.00	30.48
	2984	CG2	THR	B	493	26.067	78.953	25.372	1.00	22.03
	2985	N	GLN	B	494	30.347	78.586	26.322	1.00	35.09
	2986	CA	GLN	B	494	31.779	78.879	26.330	1.00	38.19
	2987	C	GLN	B	494	32.032	80.091	25.449	1.00	36.48
	2988	O	GLN	B	494	31.360	80.270	24.432	1.00	35.75
	2989	CB	GLN	B	494	32.581	77.696	25.775	1.00	43.09
	2990	CG	GLN	B	494	32.502	76.433	26.610	1.00	58.35
	2991	CD	GLN	B	494	32.929	76.666	28.042	1.00	65.11
	2992	OE1	GLN	B	494	34.003	77.209	28.303	1.00	71.67
	2993	NE2	GLN	B	494	32.088	76.255	28.982	1.00	71.87
	2994	N	PRO	B	495	33.002	80.939	25.828	1.00	36.89
	2995	CA	PRO	B	495	33.322	82.130	25.037	1.00	38.37
	2996	C	PRO	B	495	33.609	81.737	23.587	1.00	40.80
	2997	O	PRO	B	495	34.314	80.763	23.327	1.00	40.76
	2998	CB	PRO	B	495	34.557	82.680	25.729	1.00	37.83
	2999	CG	PRO	B	495	34.315	82.300	27.174	1.00	40.41
	3000	CD	PRO	B	495	33.809	80.884	27.061	1.00	35.81
	3001	N	ARG	B	496	33.040	82.480	22.650	1.00	42.05
	3002	CA	ARG	B	496	33.255	82.208	21.240	1.00	47.69
	3003	C	ARG	B	496	33.772	83.454	20.542	1.00	51.66

	3004	O	ARG	B	496	33.283	84.558	20.784	1.00	51.95
	3005	CB	ARG	B	496	31.954	81.751	20.584	1.00	45.81
	3006	CG	ARG	B	496	31.599	80.317	20.892	1.00	51.53
	3007	CD	ARG	B	496	30.217	79.947	20.391	1.00	53.72
	3008	NE	ARG	B	496	30.175	78.554	19.963	1.00	57.50
	3009	CZ	ARG	B	496	30.608	78.122	18.783	1.00	58.59
	3010	NH1	ARG	B	496	31.111	78.974	17.901	1.00	57.22
	3011	NH2	ARG	B	496	30.542	76.832	18.488	1.00	65.31
	3012	N	LYS	B	497	34.773	83.281	19.687	1.00	56.98
	3013	CA	LYS	B	497	35.335	84.408	18.953	1.00	61.91
	3014	C	LYS	B	497	34.301	84.867	17.955	1.00	63.97
	3015	O	LYS	B	497	33.300	84.195	17.729	1.00	64.61
	3016	CB	LYS	B	497	36.587	84.003	18.172	1.00	66.35
	3017	CG	LYS	B	497	37.848	83.781	18.987	1.00	74.14
	3018	CD	LYS	B	497	38.993	83.359	18.066	1.00	80.69
	3019	CE	LYS	B	497	40.304	83.192	18.814	1.00	84.48
	3020	NZ	LYS	B	497	41.385	82.739	17.889	1.00	88.26
	3021	N	THR	B	498	34.555	86.017	17.352	1.00	67.67
	3022	CA	THR	B	498	33.669	86.572	16.342	1.00	71.26
	3023	C	THR	B	498	34.550	87.284	15.340	1.00	73.04
	3024	O	THR	B	498	35.743	86.990	15.236	1.00	72.83
	3025	CB	THR	B	498	32.679	87.585	16.945	1.00	71.80
	3026	OG1	THR	B	498	33.392	88.555	17.721	1.00	71.58
	3027	CG2	THR	B	498	31.670	86.878	17.819	1.00	73.61
	3028	N	LYS	B	499	33.962	88.220	14.605	1.00	75.57
	3029	CA	LYS	B	499	34.705	88.993	13.620	1.00	77.62
	3030	C	LYS	B	499	35.427	90.142	14.321	1.00	77.92
	3031	O	LYS	B	499	34.791	91.096	14.768	1.00	79.19
	3032	CB	LYS	B	499	33.752	89.558	12.567	1.00	80.22
	3033	CG	LYS	B	499	33.172	88.531	11.604	1.00	81.04
	3034	CD	LYS	B	499	34.203	88.093	10.571	1.00	83.26
	3035	CE	LYS	B	499	33.569	87.232	9.487	1.00	84.81
	3036	NZ	LYS	B	499	34.545	86.864	8.425	1.00	86.04
	3037	N	GLY	B	500	36.748	90.034	14.433	1.00	76.91
	3038	CA	GLY	B	500	37.544	91.077	15.061	1.00	75.83
	3039	C	GLY	B	500	37.141	91.560	16.445	1.00	75.14
	3040	O	GLY	B	500	37.971	91.576	17.355	1.00	75.52
	3041	N	SER	B	501	35.882	91.958	16.605	1.00	73.08
	3042	CA	SER	B	501	35.370	92.468	17.875	1.00	71.65
	3043	C	SER	B	501	36.008	91.836	19.106	1.00	68.64
	3044	O	SER	B	501	36.690	92.515	19.877	1.00	71.13
	3045	CB	SER	B	501	33.854	92.279	17.953	1.00	74.43
	3046	OG	SER	B	501	33.524	90.933	18.241	1.00	80.92
	3047	N	GLY	B	502	35.786	90.540	19.290	1.00	63.14
	3048	CA	GLY	B	502	36.344	89.859	20.443	1.00	54.62
	3049	C	GLY	B	502	35.552	88.618	20.803	1.00	48.04
	3050	O	GLY	B	502	35.469	87.683	20.006	1.00	48.08
	3051	N	PHE	B	503	34.958	88.599	21.994	1.00	40.50
	3052	CA	PHE	B	503	34.189	87.427	22.408	1.00	33.81
	3053	C	PHE	B	503	32.773	87.692	22.888	1.00	28.39
	3054	O	PHE	B	503	32.408	88.811	23.244	1.00	26.35
	3055	CB	PHE	B	503	34.919	86.662	23.517	1.00	35.09
	3056	CG	PHE	B	503	36.263	86.148	23.119	1.00	34.16
	3057	CD1	PHE	B	503	37.381	86.970	23.174	1.00	35.05
	3058	CD2	PHE	B	503	36.411	84.845	22.670	1.00	35.90
	3059	CE1	PHE	B	503	38.633	86.501	22.783	1.00	36.00
	3060	CE2	PHE	B	503	37.656	84.362	22.274	1.00	40.04
	3061	CZ	PHE	B	503	38.771	85.192	22.329	1.00	38.82
	3062	N	PHE	B	504	31.975	86.633	22.884	1.00	26.16
	3063	CA	PHE	B	504	30.612	86.709	23.369	1.00	25.00
	3064	C	PHE	B	504	30.286	85.418	24.096	1.00	26.57
	3065	O	PHE	B	504	30.892	84.379	23.833	1.00	26.73

	3066	CB	PHE	B	504	29.616	86.960	22.242	1.00	22.46
45	3067	CG	PHE	B	504	29.330	85.766	21.382	1.00	27.70
	3068	CD1	PHE	B	504	28.260	84.926	21.667	1.00	28.94
	3069	CD2	PHE	B	504	30.086	85.517	20.243	1.00	31.34
	3070	CE1	PHE	B	504	27.938	83.857	20.827	1.00	30.08
	3071	CE2	PHE	B	504	29.772	84.449	19.396	1.00	32.65
50	3072	CZ	PHE	B	504	28.691	83.621	19.697	1.00	32.80
	3073	N	VAL	B	505	29.330	85.509	25.015	1.00	23.68
	3074	CA	VAL	B	505	28.895	84.389	25.814	1.00	24.67
	3075	C	VAL	B	505	27.385	84.559	26.028	1.00	23.86
	3076	O	VAL	B	505	26.875	85.672	26.051	1.00	21.24
55	3077	CB	VAL	B	505	29.674	84.392	27.161	1.00	27.95
	3078	CG1	VAL	B	505	29.136	85.466	28.080	1.00	25.61
	3079	CG2	VAL	B	505	29.643	83.042	27.786	1.00	33.51
	3080	N	PHE	B	506	26.664	83.454	26.141	1.00	26.20
	3081	CA	PHE	B	506	25.218	83.514	26.346	1.00	26.10
5	3082	C	PHE	B	506	24.855	82.754	27.621	1.00	24.83
	3083	O	PHE	B	506	25.369	81.672	27.859	1.00	25.52
	3084	CB	PHE	B	506	24.496	82.875	25.161	1.00	28.18
	3085	CG	PHE	B	506	23.007	82.842	25.303	1.00	35.33
	3086	CD1	PHE	B	506	22.245	83.980	25.080	1.00	42.56
10	3087	CD2	PHE	B	506	22.359	81.663	25.657	1.00	40.04
	3088	CE1	PHE	B	506	20.854	83.940	25.208	1.00	44.70
	3089	CE2	PHE	B	506	20.977	81.613	25.789	1.00	40.54
	3090	CZ	PHE	B	506	20.223	82.749	25.564	1.00	42.12
	3091	N	SER	B	507	23.961	83.310	28.427	1.00	24.69
15	3092	CA	SER	B	507	23.550	82.659	29.674	1.00	24.73
	3093	C	SER	B	507	22.022	82.535	29.745	1.00	26.40
	3094	O	SER	B	507	21.308	83.487	29.491	1.00	25.99
	3095	CB	SER	B	507	24.079	83.449	30.879	1.00	22.19
	3096	OG	SER	B	507	23.653	82.860	32.091	1.00	30.30
20	3097	N	ARG	B	508	21.538	81.345	30.091	1.00	26.98
	3098	CA	ARG	B	508	20.104	81.055	30.187	1.00	25.95
	3099	C	ARG	B	508	19.689	80.749	31.637	1.00	24.97
	3100	O	ARG	B	508	20.350	79.979	32.315	1.00	24.35
	3101	CB	ARG	B	508	19.799	79.845	29.310	1.00	21.97
25	3102	CG	ARG	B	508	18.365	79.351	29.344	1.00	25.32
	3103	CD	ARG	B	508	18.228	78.126	28.444	1.00	25.67
	3104	NE	ARG	B	508	16.842	77.702	28.312	1.00	36.00
	3105	CZ	ARG	B	508	16.243	76.843	29.128	1.00	36.06
	3106	NH1	ARG	B	508	16.918	76.307	30.137	1.00	34.19
30	3107	NH2	ARG	B	508	14.967	76.538	28.943	1.00	34.70
	3108	N	LEU	B	509	18.583	81.331	32.099	1.00	26.44
	3109	CA	LEU	B	509	18.121	81.108	33.479	1.00	28.45
	3110	C	LEU	B	509	16.627	80.806	33.560	1.00	28.87
	3111	O	LEU	B	509	15.803	81.707	33.401	1.00	30.99
35	3112	CB	LEU	B	509	18.423	82.341	34.342	1.00	27.28
	3113	CG	LEU	B	509	17.867	82.330	35.779	1.00	31.90
	3114	CD1	LEU	B	509	18.615	81.316	36.647	1.00	29.48
	3115	CD2	LEU	B	509	18.001	83.714	36.368	1.00	28.89
	3116	N	GLU	B	510	16.277	79.546	33.812	1.00	31.92
40	3117	CA	GLU	B	510	14.872	79.152	33.911	1.00	34.67
	3118	C	GLU	B	510	14.310	79.595	35.255	1.00	36.35
	3119	O	GLU	B	510	14.948	79.401	36.288	1.00	34.66
	3120	CB	GLU	B	510	14.725	77.630	33.757	1.00	41.07
	3121	CG	GLU	B	510	15.217	77.090	32.404	1.00	54.35
45	3122	CD	GLU	B	510	14.925	75.603	32.189	1.00	58.86
	3123	OE1	GLU	B	510	15.236	74.789	33.087	1.00	61.22
	3124	OE2	GLU	B	510	14.393	75.251	31.111	1.00	61.34
	3125	N	VAL	B	511	13.121	80.194	35.248	1.00	36.50
	3126	CA	VAL	B	511	12.531	80.665	36.494	1.00	38.05
50	3127	C	VAL	B	511	11.084	80.230	36.692	1.00	42.41

	3128	O	VAL	B	511	10.395	79.856	35.732	1.00	41.92
	3129	CB	VAL	B	511	12.588	82.197	36.592	1.00	31.84
	3130	CG1	VAL	B	511	14.015	82.673	36.431	1.00	32.42
	3131	CG2	VAL	B	511	11.687	82.813	35.547	1.00	26.87
	3132	N	THR	B	512	10.633	80.290	37.946	1.00	43.58
	3133	CA	THR	B	512	9.269	79.903	38.292	1.00	48.37
	3134	C	THR	B	512	8.294	80.998	37.899	1.00	50.53
	3135	O	THR	B	512	8.706	82.113	37.584	1.00	51.77
	3136	CB	THR	B	512	9.125	79.644	39.797	1.00	48.57
	3137	OG1	THR	B	512	9.460	80.834	40.519	1.00	46.96
	3138	CG2	THR	B	512	10.046	78.515	40.234	1.00	45.82
	3139	N	ARG	B	513	7.002	80.678	37.912	1.00	53.29
	3140	CA	ARG	B	513	5.971	81.648	37.556	1.00	55.54
	3141	C	ARG	B	513	6.043	82.819	38.523	1.00	55.38
	3142	O	ARG	B	513	5.859	83.977	38.138	1.00	55.22
	3143	CB	ARG	B	513	4.582	81.006	37.636	1.00	59.23
	3144	CG	ARG	B	513	3.563	81.601	36.672	1.00	65.98
	3145	CD	ARG	B	513	3.326	83.081	36.916	1.00	74.12
	3146	NE	ARG	B	513	2.773	83.742	35.735	1.00	80.97
	3147	CZ	ARG	B	513	2.403	85.019	35.687	1.00	83.64
	3148	NH1	ARG	B	513	2.516	85.791	36.760	1.00	86.02
	3149	NH2	ARG	B	513	1.927	85.528	34.557	1.00	85.44
	3150	N	ALA	B	514	6.315	82.501	39.783	1.00	55.03
	3151	CA	ALA	B	514	6.414	83.504	40.832	1.00	55.46
	3152	C	ALA	B	514	7.496	84.539	40.529	1.00	56.10
	3153	O	ALA	B	514	7.210	85.734	40.426	1.00	56.61
	3154	CB	ALA	B	514	6.692	82.825	42.173	1.00	54.05
	3155	N	GLU	B	515	8.741	84.091	40.388	1.00	55.46
	3156	CA	GLU	B	515	9.819	85.025	40.105	1.00	55.34
	3157	C	GLU	B	515	9.649	85.651	38.729	1.00	54.83
	3158	O	GLU	B	515	10.190	86.723	38.456	1.00	52.33
	3159	CB	GLU	B	515	11.187	84.335	40.232	1.00	57.76
	3160	CG	GLU	B	515	11.221	82.884	39.788	1.00	62.58
	3161	CD	GLU	B	515	12.518	82.184	40.163	1.00	63.27
	3162	OE1	GLU	B	515	13.035	82.432	41.271	1.00	64.89
	3163	OE2	GLU	B	515	13.014	81.372	39.359	1.00	66.59
	3164	N	TRP	B	516	8.884	84.992	37.866	1.00	55.79
	3165	CA	TRP	B	516	8.644	85.528	36.534	1.00	57.81
	3166	C	TRP	B	516	7.778	86.782	36.636	1.00	58.51
	3167	O	TRP	B	516	7.778	87.612	35.726	1.00	57.71
	3168	CB	TRP	B	516	7.951	84.499	35.634	1.00	61.48
	3169	CG	TRP	B	516	8.056	84.862	34.187	1.00	66.54
	3170	CD1	TRP	B	516	9.172	84.777	33.403	1.00	67.26
	3171	CD2	TRP	B	516	7.039	85.460	33.375	1.00	69.56
	3172	NE1	TRP	B	516	8.915	85.291	32.154	1.00	71.76
	3173	CE2	TRP	B	516	7.613	85.718	32.110	1.00	70.88
	3174	CE3	TRP	B	516	5.700	85.807	33.593	1.00	70.94
	3175	CZ2	TRP	B	516	6.894	86.308	31.066	1.00	73.50
	3176	CZ3	TRP	B	516	4.982	86.396	32.552	1.00	74.37
	3177	CH2	TRP	B	516	5.584	86.639	31.304	1.00	74.71
	3178	N	GLU	B	517	7.047	86.918	37.744	1.00	59.66
	3179	CA	GLU	B	517	6.191	88.085	37.972	1.00	61.72
	3180	C	GLU	B	517	7.035	89.299	38.354	1.00	59.87
	3181	O	GLU	B	517	6.606	90.441	38.196	1.00	58.60
	3182	CB	GLU	B	517	5.182	87.818	39.097	1.00	68.82
	3183	CG	GLU	B	517	4.284	86.612	38.879	1.00	80.60
	3184	CD	GLU	B	517	3.242	86.452	39.976	1.00	87.42
	3185	OE1	GLU	B	517	3.369	87.128	41.021	1.00	94.80
	3186	OE2	GLU	B	517	2.301	85.645	39.800	1.00	95.35
	3187	N	GLN	B	518	8.234	89.045	38.867	1.00	57.92

	3188	CA	GLN	B	518	9.132	90.120	39.264	1.00	55.74
	3189	C	GLN	B	518	10.416	90.057	38.436	1.00	54.32
	3190	O	GLN	B	518	11.498	90.393	38.924	1.00	52.85
	3191	CB	GLN	B	518	9.454	90.000	40.745	1.00	54.10
	3192	N	LYS	B	519	10.287	89.646	37.176	1.00	52.69
	3193	CA	LYS	B	519	11.448	89.518	36.309	1.00	52.35
	3194	C	LYS	B	519	12.206	90.819	36.159	1.00	51.69
	3195	O	LYS	B	519	13.397	90.822	35.854	1.00	49.61
	3196	CB	LYS	B	519	11.039	88.983	34.937	1.00	54.31
	3197	CG	LYS	B	519	10.205	89.912	34.088	1.00	55.80
	3198	CD	LYS	B	519	9.723	89.162	32.859	1.00	60.32
	3199	CE	LYS	B	519	8.794	90.002	32.011	1.00	64.05
	3200	NZ	LYS	B	519	8.223	89.191	30.898	1.00	70.92
	3201	N	ASP	B	520	11.511	91.924	36.388	1.00	52.66
	3202	CA	ASP	B	520	12.105	93.251	36.288	1.00	54.22
	3203	C	ASP	B	520	13.209	93.396	37.336	1.00	53.07
	3204	O	ASP	B	520	14.075	94.264	37.229	1.00	52.75
	3205	CB	ASP	B	520	11.032	94.311	36.537	1.00	61.14
	3206	CG	ASP	B	520	9.620	93.779	36.308	1.00	71.19
	3207	OD1	ASP	B	520	9.300	93.407	35.155	1.00	76.53
	3208	OD2	ASP	B	520	8.834	93.729	37.283	1.00	72.86
	3209	N	GLU	B	521	13.177	92.533	38.343	1.00	51.01
	3210	CA	GLU	B	521	14.157	92.582	39.416	1.00	50.49
	3211	C	GLU	B	521	15.394	91.714	39.201	1.00	47.73
	3212	O	GLU	B	521	16.372	91.838	39.935	1.00	48.58
	3213	CB	GLU	B	521	13.493	92.200	40.738	1.00	53.54
	3214	CG	GLU	B	521	12.427	93.177	41.199	1.00	60.11
	3215	CD	GLU	B	521	11.705	92.699	42.442	1.00	65.41
	3216	OE1	GLU	B	521	12.361	92.497	43.486	1.00	67.98
	3217	OE2	GLU	B	521	10.471	92.521	42.374	1.00	73.58
	3218	N	PHE	B	522	15.359	90.828	38.213	1.00	42.66
	3219	CA	PHE	B	522	16.519	89.985	37.963	1.00	38.90
	3220	C	PHE	B	522	17.583	90.753	37.208	1.00	35.93
	3221	O	PHE	B	522	17.276	91.579	36.345	1.00	38.85
	3222	CB	PHE	B	522	16.122	88.716	37.214	1.00	36.56
	3223	CG	PHE	B	522	15.419	87.710	38.081	1.00	39.04
	3224	CD1	PHE	B	522	14.106	87.927	38.495	1.00	42.28
	3225	CD2	PHE	B	522	16.087	86.574	38.539	1.00	36.78
	3226	CE1	PHE	B	522	13.468	87.029	39.362	1.00	44.30
	3227	CE2	PHE	B	522	15.461	85.673	39.405	1.00	40.92
	3228	CZ	PHE	B	522	14.146	85.901	39.817	1.00	39.51
	3229	N	ILE	B	523	18.837	90.492	37.555	1.00	31.27
	3230	CA	ILE	B	523	19.959	91.173	36.944	1.00	29.65
	3231	C	ILE	B	523	21.049	90.211	36.483	1.00	29.13
	3232	O	ILE	B	523	21.360	89.236	37.164	1.00	27.36
	3233	CB	ILE	B	523	20.567	92.180	37.937	1.00	34.21
	3234	CG1	ILE	B	523	19.528	93.251	38.282	1.00	37.38
	3235	CG2	ILE	B	523	21.827	92.796	37.364	1.00	34.94
	3236	CD1	ILE	B	523	19.981	94.227	39.354	1.00	38.56
	3237	N	CYS	B	524	21.610	90.498	35.311	1.00	26.34
	3238	CA	CYS	B	524	22.686	89.699	34.739	1.00	27.10
	3239	C	CYS	B	524	23.946	90.500	34.962	1.00	26.67
	3240	O	CYS	B	524	24.010	91.655	34.569	1.00	27.58
	3241	CB	CYS	B	524	22.473	89.497	33.226	1.00	24.27
	3242	SG	CYS	B	524	23.823	88.626	32.363	1.00	37.60
	3243	N	ARG	B	525	24.951	89.886	35.572	1.00	26.37
	3244	CA	ARG	B	525	26.194	90.576	35.856	1.00	26.35
	3245	C	ARG	B	525	27.419	89.887	35.304	1.00	26.72
	3246	O	ARG	B	525	27.561	88.671	35.400	1.00	29.04
	3247	CB	ARG	B	525	26.376	90.748	37.361	1.00	29.81

	3248	CG	ARG	B	525	27.713	91.393	37.728	1.00	35.40
	3249	CD	ARG	B	525	27.652	92.058	39.099	1.00	46.51
	3250	NE	ARG	B	525	27.796	91.113	40.193	1.00	50.77
	3251	CZ	ARG	B	525	27.461	91.379	41.451	1.00	55.09
	3252	NH1	ARG	B	525	26.951	92.565	41.763	1.00	54.58
	3253	NH2	ARG	B	525	27.650	90.464	42.397	1.00	56.77
	3254	N	ALA	B	526	28.311	90.680	34.731	1.00	25.38
	3255	CA	ALA	B	526	29.528	90.142	34.180	1.00	25.38
	3256	C	ALA	B	526	30.721	90.728	34.925	1.00	25.99
	3257	O	ALA	B	526	30.751	91.933	35.210	1.00	25.50
	3258	CB	ALA	B	526	29.629	90.484	32.696	1.00	25.98
	3259	N	VAL	B	527	31.684	89.872	35.259	1.00	23.84
	3260	CA	VAL	B	527	32.895	90.333	35.902	1.00	25.15
	3261	C	VAL	B	527	33.972	90.078	34.880	1.00	26.30
	3262	O	VAL	B	527	34.119	88.958	34.394	1.00	26.20
	3263	CB	VAL	B	527	33.235	89.557	37.177	1.00	24.43
	3264	CG1	VAL	B	527	34.588	89.990	37.661	1.00	26.95
	3265	CG2	VAL	B	527	32.191	89.819	38.251	1.00	28.13
	3266	N	HIS	B	528	34.738	91.115	34.569	1.00	26.24
	3267	CA	HIS	B	528	35.772	91.028	33.564	1.00	29.14
	3268	C	HIS	B	528	36.822	92.102	33.805	1.00	31.86
	3269	O	HIS	B	528	36.509	93.216	34.239	1.00	31.05
	3270	CB	HIS	B	528	35.121	91.172	32.179	1.00	29.03
	3271	CG	HIS	B	528	36.077	91.082	31.035	1.00	29.34
	3272	ND1	HIS	B	528	36.934	92.109	30.696	1.00	33.33
	3273	CD2	HIS	B	528	36.317	90.090	30.144	1.00	28.93
	3274	CE1	HIS	B	528	37.655	91.755	29.651	1.00	26.07
	3275	NE2	HIS	B	528	37.302	90.530	29.295	1.00	32.19
	3276	N	GLU	B	529	38.064	91.757	33.501	1.00	34.08
	3277	CA	GLU	B	529	39.207	92.636	33.676	1.00	39.76
	3278	C	GLU	B	529	39.110	94.037	33.066	1.00	41.50
	3279	O	GLU	B	529	39.410	95.020	33.740	1.00	41.48
	3280	CB	GLU	B	529	40.462	91.959	33.122	1.00	43.03
	3281	CG	GLU	B	529	41.665	92.898	33.086	1.00	56.19
	3282	CD	GLU	B	529	42.827	92.361	32.274	1.00	62.66
	3283	OE1	GLU	B	529	43.812	93.111	32.093	1.00	63.52
	3284	OE2	GLU	B	529	42.758	91.198	31.819	1.00	65.43
	3285	N	ALA	B	530	38.703	94.121	31.800	1.00	42.51
	3286	CA	ALA	B	530	38.622	95.399	31.094	1.00	46.03
	3287	C	ALA	B	530	37.495	96.331	31.504	1.00	49.29
	3288	O	ALA	B	530	37.447	97.476	31.056	1.00	50.87
	3289	CB	ALA	B	530	38.557	95.157	29.587	1.00	39.71
	3290	N	ALA	B	531	36.595	95.849	32.352	1.00	52.89
	3291	CA	ALA	B	531	35.467	96.651	32.798	1.00	56.14
	3292	C	ALA	B	531	35.801	97.570	33.976	1.00	59.66
	3293	O	ALA	B	531	35.357	97.342	35.096	1.00	61.00
	3294	CB	ALA	B	531	34.305	95.736	33.162	1.00	52.83
	3295	N	SER	B	532	36.588	98.608	33.730	1.00	63.07
	3296	CA	SER	B	532	36.927	99.544	34.795	1.00	66.03
	3297	C	SER	B	532	35.822	100.594	34.850	1.00	66.08
	3298	O	SER	B	532	35.317	101.031	33.814	1.00	65.35
	3299	CB	SER	B	532	38.270	100.216	34.507	1.00	68.98
	3300	OG	SER	B	532	38.184	101.074	33.384	1.00	74.64
	3301	N	PRO	B	533	35.427	101.019	36.057	1.00	66.51
	3302	CA	PRO	B	533	35.887	100.669	37.404	1.00	65.99
	3303	C	PRO	B	533	35.374	99.349	37.983	1.00	63.48
	3304	O	PRO	B	533	34.327	98.840	37.582	1.00	64.33
	3305	CB	PRO	B	533	35.397	101.843	38.227	1.00	69.06
	3306	CG	PRO	B	533	34.044	102.061	37.629	1.00	71.08
	3307	CD	PRO	B	533	34.358	102.030	36.137	1.00	70.23
	3308	N	SER	B	534	36.134	98.817	38.935	1.00	59.21
	3309	CA	SER	B	534	35.796	97.591	39.648	1.00	55.01

	3310	C	SER	B	534	35.452	96.326	38.852	1.00	50.27
	3311	O	SER	B	534	34.725	95.470	39.347	1.00	48.58
	3312	CB	SER	B	534	34.666	97.894	40.625	1.00	58.20
	3313	OG	SER	B	534	33.587	98.526	39.962	1.00	63.36
	3314	N	GLN	B	535	35.984	96.213	37.639	1.00	44.89
	3315	CA	GLN	B	535	35.771	95.057	36.770	1.00	42.88
	3316	C	GLN	B	535	34.395	94.406	36.823	1.00	41.55
	3317	O	GLN	B	535	34.279	93.181	36.806	1.00	40.80
	3318	CB	GLN	B	535	36.831	93.967	37.020	1.00	37.08
	3319	CG	GLN	B	535	37.869	94.298	38.044	1.00	47.40
	3320	CD	GLN	B	535	38.684	95.499	37.669	1.00	44.36
	3321	OE1	GLN	B	535	38.862	96.407	38.475	1.00	47.59
	3322	NE2	GLN	B	535	39.185	95.521	36.436	1.00	54.70
	3323	N	THR	B	536	33.348	95.213	36.874	1.00	39.97
	3324	CA	THR	B	536	32.012	94.650	36.893	1.00	40.62
	3325	C	THR	B	536	31.025	95.487	36.077	1.00	37.57
	3326	O	THR	B	536	31.042	96.707	36.125	1.00	40.85
	3327	CB	THR	B	536	31.508	94.463	38.353	1.00	42.38
	3328	OG1	THR	B	536	30.112	94.142	38.337	1.00	44.59
	3329	CG2	THR	B	536	31.730	95.719	39.168	1.00	49.65
	3330	N	VAL	B	537	30.190	94.812	35.299	1.00	35.29
	3331	CA	VAL	B	537	29.182	95.453	34.468	1.00	31.25
	3332	C	VAL	B	537	27.922	94.604	34.563	1.00	29.01
	3333	O	VAL	B	537	27.985	93.382	34.401	1.00	30.11
	3334	CB	VAL	B	537	29.604	95.494	32.983	1.00	34.80
	3335	CG1	VAL	B	537	28.516	96.148	32.161	1.00	35.52
	3336	CG2	VAL	B	537	30.888	96.259	32.822	1.00	37.19
	3337	N	GLN	B	538	26.780	95.235	34.808	1.00	26.73
	3338	CA	GLN	B	538	25.533	94.493	34.933	1.00	26.74
	3339	C	GLN	B	538	24.329	95.224	34.368	1.00	27.53
	3340	O	GLN	B	538	24.351	96.431	34.198	1.00	29.89
	3341	CB	GLN	B	538	25.265	94.176	36.400	1.00	28.48
	3342	CG	GLN	B	538	24.976	95.392	37.266	1.00	25.88
	3343	CD	GLN	B	538	24.747	95.005	38.722	1.00	28.51
	3344	OE1	GLN	B	538	25.498	94.210	39.290	1.00	31.66
	3345	NE2	GLN	B	538	23.715	95.565	39.328	1.00	27.39
	3346	N	ARG	B	539	23.266	94.487	34.087	1.00	28.05
	3347	CA	ARG	B	539	22.070	95.107	33.565	1.00	30.72
	3348	C	ARG	B	539	20.858	94.312	33.986	1.00	31.33
	3349	O	ARG	B	539	20.897	93.083	34.023	1.00	32.42
	3350	CB	ARG	B	539	22.137	95.180	32.039	1.00	36.30
	3351	CG	ARG	B	539	21.124	96.112	31.414	1.00	45.60
	3352	CD	ARG	B	539	21.771	96.859	30.270	1.00	57.97
	3353	NE	ARG	B	539	23.009	97.482	30.729	1.00	69.46
	3354	CZ	ARG	B	539	23.855	98.147	29.950	1.00	78.18
	3355	NH1	ARG	B	539	23.604	98.284	28.653	1.00	83.01
	3356	NH2	ARG	B	539	24.959	98.673	30.470	1.00	81.89
	3357	N	ALA	B	540	19.782	95.022	34.301	1.00	31.92
	3358	CA	ALA	B	540	18.546	94.393	34.717	1.00	34.50
	3359	C	ALA	B	540	17.826	93.909	33.466	1.00	36.68
	3360	O	ALA	B	540	18.068	94.410	32.361	1.00	34.62
	3361	CB	ALA	B	540	17.693	95.391	35.479	1.00	33.91
	3362	N	VAL	B	541	16.974	92.906	33.640	1.00	39.73
	3363	CA	VAL	B	541	16.214	92.346	32.528	1.00	44.47
	3364	C	VAL	B	541	15.351	93.436	31.882	1.00	46.91
	3365	O	VAL	B	541	14.476	94.005	32.527	1.00	44.53
	3366	CB	VAL	B	541	15.305	91.185	33.010	1.00	42.49
	3367	CG1	VAL	B	541	14.242	90.885	31.970	1.00	47.96
	3368	CG2	VAL	B	541	16.140	89.945	33.269	1.00	42.43
	3369	N	SER	B	542	15.603	93.731	30.611	1.00	52.25
	3370	CA	SER	B	542	14.829	94.760	29.926	1.00	60.05
	3371	C	SER	B	542	13.426	94.226	29.679	1.00	64.25

	3372	O	SER	B	542	13.247	93.050	29.357	1.00	65.22
	3373	CB	SER	B	542	15.490	95.157	28.600	1.00	60.43
	3374	OG	SER	B	542	15.524	94.070	27.696	1.00	65.30
	3375	N	VAL	B	543	12.432	95.090	29.844	1.00	68.19
	3376	CA	VAL	B	543	11.043	94.694	29.656	1.00	72.45
	3377	C	VAL	B	543	10.277	95.772	28.898	1.00	74.32
	3378	O	VAL	B	543	9.621	96.630	29.497	1.00	75.99
	3379	CB	VAL	B	543	10.353	94.452	31.016	1.00	74.41
	3380	CG1	VAL	B	543	8.895	94.070	30.801	1.00	76.37
	3381	CG2	VAL	B	543	11.086	93.367	31.782	1.00	75.78
	3382	O	HOH	B	1	28.242	81.091	34.909	1.00	54.75
	3383	O	HOH	B	2	20.156	98.063	34.554	1.00	37.27
	3384	O	HOH	B	3	9.164	79.181	26.395	1.00	46.90
	3385	O	HOH	B	4	40.362	78.148	37.537	1.00	44.93
	3386	O	HOH	B	5	26.513	97.015	29.107	1.00	46.77
	3387	O	HOH	B	6	24.671	83.376	40.011	1.00	40.32
	3388	O	HOH	B	7	50.797	88.328	45.010	1.00	50.21
	3389	O	HOH	B	8	30.596	75.260	16.415	1.00	61.75
	3390	O	HOH	B	9	39.623	81.063	40.390	1.00	39.17
	3391	O	HOH	B	10	10.819	88.759	44.203	1.00	64.36
	3392	O	HOH	B	11	43.896	82.650	46.479	1.00	45.74
	3393	O	HOH	B	12	40.405	77.131	40.006	1.00	39.34
	3394	O	HOH	B	13	28.630	51.829	41.383	1.00	56.15
	3395	O	HOH	B	14	18.197	77.472	34.045	1.00	46.48
	3396	O	HOH	B	15	29.246	81.729	23.290	1.00	36.55
	3397	O	HOH	B	16	27.005	76.944	32.905	1.00	48.95
	3398	O	HOH	B	17	46.365	79.161	30.402	1.00	50.90
	3399	O	HOH	B	18	29.027	56.778	36.404	1.00	58.83
	3400	O	HOH	B	19	32.617	59.584	31.846	1.00	61.24
	3401	O	HOH	B	20	46.447	87.589	46.492	1.00	58.37
	3402	O	HOH	B	21	37.888	95.014	40.873	1.00	57.48
	3403	O	HOH	B	22	55.424	66.383	26.960	1.00	60.62
	3404	O	HOH	B	23	49.953	85.610	35.164	1.00	49.14
	3405	O	HOH	B	24	0.662	87.508	40.326	1.00	63.67
	3406	O	HOH	B	25	19.011	94.187	29.591	1.00	40.50
	3407	O	HOH	B	26	43.242	49.660	46.237	1.00	58.12
	3408	O	HOH	B	27	40.629	78.744	31.911	1.00	52.34
	3409	O	HOH	B	28	40.803	72.686	34.647	1.00	52.41
	3410	O	HOH	B	29	-1.434	81.662	24.774	1.00	63.47
	3411	O	HOH	B	30	29.558	77.458	32.128	1.00	56.91
	3412	O	HOH	B	31	40.590	70.716	43.907	1.00	49.06
	3413	O	HOH	B	32	23.070	95.434	42.368	1.00	59.31
	3414	O	HOH	B	33	58.388	76.819	41.695	1.00	51.40
	3415	O	HOH	B	34	50.954	79.227	44.916	1.00	49.71
	3416	O	HOH	B	35	34.068	54.729	35.446	1.00	64.98
	3417	O	HOH	B	36	29.928	90.630	44.684	1.00	55.97
	3418	O	HOH	B	37	29.718	98.417	28.749	1.00	56.10
	3419	O	HOH	B	38	34.139	96.711	23.956	1.00	48.69
	3420	O	HOH	B	39	38.006	89.010	17.278	1.00	58.57
	3421	O	HOH	B	40	52.915	67.142	28.195	1.00	54.81
	3422	O	HOH	B	41	41.555	51.194	38.581	1.00	65.02
	3423	O	HOH	B	42	52.498	94.849	41.604	1.00	60.95
	3424	O	HOH	B	43	23.412	53.599	37.661	1.00	59.29
	3425	O	HOH	B	44	28.241	88.615	44.746	1.00	64.70
	3426	O	HOH	B	45	54.871	85.305	45.726	1.00	57.91
	3427	O	HOH	B	46	9.818	81.648	43.286	1.00	54.20
	3428	O	HOH	B	47	26.359	91.470	45.088	1.00	59.40
	3429	O	HOH	B	48	28.072	63.227	38.869	1.00	61.07
	3430	O	HOH	B	49	45.277	55.789	32.757	1.00	62.77
	3431	O	HOH	B	50	44.758	73.013	29.503	1.00	54.90
	3432	O	HOH	B	51	38.266	78.900	44.091	1.00	59.03
	3433	O	HOH	B	52	8.212	78.463	34.558	1.00	57.55

	3434	O	HOH	B	53	1.381	85.874	28.805	1.00	55.02
	3435	O	HOH	B	54	26.806	78.029	35.293	1.00	62.62
	3436	O	HOH	B	55	12.447	95.162	25.458	1.00	64.18
	3437	O	HOH	B	56	3.811	85.411	25.179	1.00	57.80
	3438	O	HOH	B	57	29.871	60.364	33.052	1.00	68.28
	3439	O	HOH	B	58	19.470	76.874	31.345	1.00	42.77
	3440	O	HOH	B	59	43.684	89.839	24.236	1.00	49.12
	3441	O	HOH	B	60	8.499	86.927	28.688	1.00	60.00
	3442	O	HOH	B	61	42.759	54.014	38.123	1.00	66.82
	3443	O	HOH	B	62	57.282	92.935	37.270	1.00	61.58
	3444	O	HOH	B	63	35.759	94.606	20.953	1.00	54.56
	3445	O	HOH	B	64	55.504	71.596	38.010	1.00	52.20
	3446	O	HOH	B	65	51.524	82.672	43.463	1.00	63.55
	3447	O	HOH	B	66	25.162	92.476	24.637	1.00	49.41
	3448	O	HOH	B	67	20.866	91.104	50.882	1.00	59.74
	3449	O	HOH	B	68	21.567	72.397	38.063	1.00	61.59
	3450	O	HOH	B	69	34.917	80.449	18.554	1.00	58.32
	3451	O	HOH	B	70	58.059	62.072	40.018	1.00	67.46
	3452	O	HOH	B	71	46.678	76.624	50.973	1.00	56.29
	3453	O	HOH	B	72	47.970	66.515	43.658	1.00	57.89
	3454	O	HOH	B	73	58.976	70.892	35.943	1.00	61.84
	3455	O	HOH	B	74	37.925	102.300	36.267	1.00	70.53
	3456	O	HOH	B	75	35.095	82.009	30.623	1.00	53.22
	3457	O	HOH	B	76	48.950	89.607	45.995	1.00	60.73
	3458	O	HOH	B	77	51.049	54.014	41.456	1.00	64.35
	3459	O	HOH	B	78	9.614	90.974	28.382	1.00	59.27
	3460	O	HOH	B	79	30.892	81.866	34.924	1.00	53.70
	3461	O	HOH	B	80	8.623	88.500	43.305	1.00	60.32
	3462	O	HOH	B	81	37.845	96.067	20.364	1.00	56.40
	3463	O	HOH	B	82	38.754	86.712	18.621	1.00	62.11
	3464	O	HOH	B	83	33.854	61.761	30.984	1.00	57.66
	3465	O	HOH	B	84	31.092	97.083	24.789	1.00	61.70
	3466	O	HOH	B	85	55.604	63.730	25.209	1.00	61.38
	3467	O	HOH	B	86	10.681	91.038	44.382	1.00	67.86
	3468	O	HOH	B	87	8.631	76.809	27.264	1.00	61.99
	3469	O	HOH	B	88	27.366	82.163	39.549	1.00	54.45
	3470	O	HOH	B	89	25.286	75.986	42.777	1.00	57.86
	3471	O	HOH	B	90	37.707	77.054	41.662	1.00	58.43
	3472	O	HOH	B	91	32.692	58.560	34.055	1.00	67.78
	3473	O	HOH	B	92	53.944	63.193	28.977	1.00	65.22
	3474	O	HOH	B	93	39.865	81.851	49.172	1.00	60.31
	3475	O	HOH	B	94	31.308	61.582	30.906	1.00	61.54
	3476	O	HOH	B	95	59.514	93.999	36.788	1.00	67.64
	3477	O	HOH	B	96	39.447	99.425	29.592	1.00	56.59
	3478	O	HOH	B	97	58.449	74.096	43.103	1.00	64.62
	3479	O	HOH	B	98	29.674	63.288	40.778	1.00	66.03
	3480	O	HOH	B	99	48.458	74.578	28.945	1.00	62.65
	3481	O	HOH	B	100	1.217	87.605	43.348	1.00	63.95
	3482	O	HOH	B	101	18.899	94.884	51.591	1.00	63.86
	3483	O	HOH	B	102	32.969	77.837	30.721	1.00	62.58
	3484	O	HOH	B	103	0.563	90.219	39.830	1.00	58.40
	3485	O	HOH	B	104	26.801	57.949	31.582	1.00	61.34
	3486	O	HOH	B	105	11.041	70.673	37.151	1.00	65.87
	3487	O	HOH	B	106	22.839	96.513	26.321	1.00	61.27
	3488	O	HOH	B	107	51.734	82.918	46.361	1.00	67.17
	3489	O	HOH	B	108	47.037	68.251	48.363	1.00	54.90
	3490	O	HOH	B	109	7.726	80.618	44.317	1.00	66.23
	3491	O	HOH	B	110	32.588	73.719	18.127	1.00	59.96
	3492	O	HOH	B	111	44.611	57.647	45.310	1.00	64.92
	3493	O	HOH	B	112	32.288	63.471	36.999	1.00	65.68
	3494	O	HOH	B	113	47.059	68.725	45.458	1.00	61.47
	3495	O	HOH	B	114	52.648	70.274	44.235	1.00	60.20

	3496	O	HOH	B	115	28.226	99.464	26.888	1.00	59.29
	3497	O	HOH	B	116	10.671	79.859	28.221	1.00	53.05
	3498	O	HOH	B	117	47.224	51.238	37.567	1.00	69.15
	3499	O	HOH	B	118	2.077	82.274	29.937	1.00	62.28
	3500	O	HOH	B	119	21.625	99.622	31.504	1.00	59.61
	3501	O	HOH	B	120	51.385	72.528	46.379	1.00	61.94
	3502	O	HOH	B	121	60.228	68.403	35.257	1.00	64.45
	3503	O	HOH	B	122	40.261	93.766	43.138	1.00	63.01
	3504	O	HOH	B	123	25.735	89.468	46.487	1.00	59.29
	3505	O	HOH	B	124	31.385	92.796	46.304	1.00	61.69
	3506	O	HOH	B	125	33.401	99.434	35.006	1.00	69.10
	3507	O	HOH	B	126	53.684	58.928	43.989	1.00	61.79
	3508	O	HOH	B	127	48.916	83.660	48.343	1.00	63.74
	3509	O	HOH	B	128	32.974	85.797	6.578	1.00	67.04
	3510	O	HOH	B	129	2.491	77.598	35.303	1.00	62.20
	3511	O	HOH	B	130	39.071	89.336	19.546	1.00	66.48
	3512	O	HOH	B	131	33.906	66.916	41.602	1.00	70.79
	3513	O	HOH	B	132	7.009	74.725	27.690	1.00	72.41
	3514	O	HOH	B	133	41.213	85.156	25.009	1.00	62.09
	3515	O	HOH	B	134	53.407	88.641	45.536	1.00	61.32
	3516	O	HOH	B	135	61.105	61.893	39.131	1.00	68.49
	3517	O	HOH	B	136	54.402	78.303	50.147	1.00	69.04
	3518	O	HOH	B	137	58.078	60.598	38.009	1.00	63.49
	3519	O	HOH	B	138	23.599	84.930	47.731	1.00	53.37
	3520	O	HOH	B	139	5.249	86.853	27.014	1.00	59.07
	3521	O	HOH	B	140	58.796	62.599	31.318	1.00	65.35
	3522	O	HOH	B	141	50.703	49.006	36.896	1.00	67.74
	3523	O	HOH	B	142	11.022	88.620	46.640	1.00	67.40
	3524	O	HOH	B	143	37.589	71.107	41.445	1.00	64.43
	3525	O	HOH	B	144	17.187	98.039	48.494	1.00	67.27
	3526	O	HOH	B	145	30.164	50.230	40.408	1.00	70.07

As used herein, an atomic coordinate, also referred to herein as a structure coordinate or coordinate, is a mathematical coordinate derived from mathematical equations related to the patterns obtained on diffraction of X-rays by the atoms of a protein or complex crystal. The diffraction data are typically used to calculate an electron density map, which is used to establish the positions of the individual atoms within the unit cell of the crystal. A model that substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3 includes not only models that literally represent the coordinates but also models representing a coordinate transformation of such atomic coordinates, for example, by changing the spatial orientation of the coordinates.

The present invention also includes a 3-D model that is a modification of a 3-D model that substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3. As used herein, a modification, also referred to herein as a model modification, is a model that represents an antibody Fc region that binds to a Fc receptor protein. A model modification includes, but is not limited to: a refinement of the model that substantially represents the atomic coordinates specified in Table 1, Table 2 or Table 3; a model representing any FcR-binding fragment of an antibody having the atomic coordinates specified in Table 1, Table 2 or Table 3; a model based on other Fc-Cε3/Cε4 crystals, such as a model based on a crystal disclosed in the Examples; a model produced using homology modeling techniques to, for example, incorporate all or any part of the amino acid sequence of another Fc region into a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 2 or Table 3 or incorporate all or any part of the amino acid sequence of a Fc-Cε3/Cε4 into a 3-D model of another antibody; and a modification representing a Fc region that has an altered function, which preferably can be used to design a mutein with an improved function compared to an unmodified protein. As used herein, the term unmodified protein refers to a protein that has not been intentionally subjected to either random or site-directed (i.e., targeted) mutagenesis. While not being bound by theory, it is believed that the flexibility of the Cε3 and Cε4 chains of the Fc region of IgE which allows the formation of open (receptor-bound) and closed conformations, can also lead to other dynamic

conformations, all of which are included in the present invention. Such flexibility is also a target for identification of development of compounds to inhibit binding of IgE to its receptor. In one embodiment, the distance between two Cε3 domains of a Fc region of the present invention ranges from about 10 angstroms to about 25 angstroms. In another embodiment, the distance between two Cε3 domains of a Fc region of the present invention ranges from about 20 angstroms to about 40 angstroms, with a range of from about 20 to about 30 angstroms being preferred.

A model of the present invention can be represented in a variety of forms including, but not limited to, listing the coordinates of all atoms comprising the model, providing a physical 3-D model, imaging the model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of the model, for example by extracting coordinates from a picture or placing a similar immunoglobulin domain into the 3-D model of a human Fc-Cε3/Cε4$_{222}$ protein having SEQ ID NO:2 and deriving a model of the similar domain. Physical 3-D models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, Biosym Technologies, San Diego, CA, Tripos, Inc., and Molecular Simulations Inc. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Hard copies include both motion and still pictures. Computer screen images and pictures of the model can be visualized in a number of formats including, but not limited to, electron density maps, ribbon diagrams, space-filling representations, α carbon traces, topology diagrams, lists of interatomic vectors, phi/psi/chi angle representations of the coordinates, and contact maps, examples of some of which are in the Figs. Representations of the model can include the entire model or portions thereof. A model can also be represented in a database.

A model of the present invention also defines the space surrounding that model. Such a space can be represented as a mold, or alpha-space, that can be used to predict the shape of a compound that inhibits the binding of a FcR and antibody.

In one embodiment, a model of the present invention identifies the solvent accessibility of amino acid residues of the corresponding proteins in the complex. The solvent accessibilities of the amino acids in PhFc-Cε3/Cε4$_{1\text{-}222}$ are indicated in Table 4.

Table 4. IgE-Fc Residue Exposure

Surface plot for:
structure file= 7_more_easy.mtf
coordinate set= 7_more_easy.pdb

segid	resid	resname	average accessible area residue	mainchain	sidechain
A	336	VAL	11.0355	10.7157	11.4619
A	337	SER	6.6644	0.9102	18.1728
A	338	ALA	1.5503	1.9379	0.0000
A	339	TYR	8.1765	1.1049	11.7123
A	340	LEU	3.6795	7.1662	0.1928
A	341	SER	10.1371	1.1968	28.0177
A	342	ARG	6.2194	3.9259	7.5300
A	343	PRO	1.0168	1.4058	0.4982
A	344	SER	7.7961	2.0652	19.2580
A	345	PRO	1.3218	0.0070	3.0748
A	346	PHE	4.9773	0.0000	7.8215
A	347	ASP	3.9717	0.0000	7.9435
A	348	LEU	2.0606	0.7880	3.3332
A	349	PHE	4.1860	4.1923	4.1824
A	350	ILE	8.0920	2.3463	13.8377
A	351	ARG	12.2182	6.3068	15.5962
A	352	LYS	15.4391	4.6705	24.0540
A	353	SER	8.3827	1.7463	21.6553
A	354	PRO	0.3971	0.3072	0.5168
A	355	THR	5.7285	1.2045	11.7605
A	356	ILE	0.1440	0.2879	0.0000
A	357	THR	5.3215	0.3410	11.9621
A	358	CYS	0.0000	0.0000	0.0000
A	359	LEU	3.5251	0.0000	7.0503
A	360	VAL	0.5274	0.0632	1.1465
A	361	VAL	3.5236	0.1093	8.0760
A	362	ASP	1.8760	0.2987	3.4534
A	363	ALA	20.1207	10.3102	59.3628
A	364	ALA	15.4855	4.7737	58.3324
A	365	PRO	8.8456	4.2563	14.9647
A	366	ALA	19.4281	10.6196	54.6617
A	367	LYS	14.1954	9.3656	18.0592
A	368	GLY	19.0191	19.0191	0.0000
A	369	ALA	13.5479	3.8042	52.5228
A	370	VAL	1.9022	0.2211	4.1436
A	371	ASN	9.8425	0.1360	19.5491
A	372	LEU	3.3729	6.1984	0.5473
A	373	THR	11.0885	1.1749	24.3065
A	374	TRP	1.6039	3.8874	0.6904
A	375	SER	8.4426	0.6753	23.9772
A	376	ARG	3.0964	1.9387	3.7580
A	377	ALA	15.7221	11.6308	32.0872
A	378	SER	11.3325	9.7475	14.5025
A	379	GLY	16.4108	16.4108	0.0000
A	380	LYS	13.6283	1.9326	22.9849
A	381	PRO	15.4265	3.6481	31.1310
A	382	VAL	7.3416	6.0250	9.0971
A	383	ASN	11.3782	3.3857	19.3706

	A	384	HIS	17.2932	3.2244	26.6723
	A	385	SER	9.0295	7.7970	11.4946
	A	386	THR	10.4147	0.8671	23.1449
	A	387	ARG	8.9842	6.7673	10.2510
5	A	388	LYS	13.1006	1.8914	22.0680
	A	389	GLU	12.0438	8.6316	14.7736
	A	390	ALA	12.8310	2.6317	53.6284
	A	391	ALA	26.6304	21.5969	46.7642
	A	397	LEU	7.6007	6.7288	8.4727
10	A	398	THR	5.6519	0.0606	13.1069
	A	399	VAL	0.3919	0.0000	0.9144
	A	400	THR	3.3881	0.0000	7.9056
	A	401	SER	0.6660	0.0000	1.9979
	A	402	THR	3.4801	0.2334	7.8090
15	A	403	LEU	0.1292	0.0003	0.2581
	A	404	PRO	8.0051	0.8129	17.5947
	A	405	VAL	1.7566	3.0741	0.0000
	A	406	GLY	7.5226	7.5226	0.0000
	A	407	THR	7.4670	1.2753	15.7226
20	A	408	ALA	11.6207	1.1130	53.6516
	A	409	ASP	7.3957	0.7299	14.0615
	A	410	TRP	0.6616	0.0000	0.9263
	A	411	ILE	12.9785	6.2633	19.6936
	A	412	GLU	16.8133	9.6352	22.5559
25	A	413	GLY	9.4666	9.4666	0.0000
	A	414	GLU	2.5510	2.5156	2.5794
	A	415	THR	5.9752	0.0898	13.8224
	A	416	TYR	0.5074	0.0226	0.7498
	A	417	GLN	7.2197	0.0821	12.9297
30	A	418	CYS	0.0003	0.0000	0.0009
	A	419	ALA	5.4324	0.0002	27.1613
	A	420	VAL	0.0672	0.1174	0.0002
	A	421	THR	9.2655	0.3477	21.1559
	A	422	ALA	3.5044	2.8442	6.1452
35	A	423	PRO	8.5866	10.2103	6.4216
	A	424	ALA	8.3566	3.5672	27.5142
	A	425	LEU	11.7212	8.7651	14.6773
	A	426	PRO	17.7261	10.5785	27.2562
	A	427	ARG	17.5755	2.8707	25.9782
40	A	428	ALA	9.8149	5.3119	27.8269
	A	429	LEU	6.4318	0.7950	12.0687
	A	430	MET	15.6753	5.2815	26.0691
	A	431	ARG	8.2369	1.4606	12.1090
	A	432	SER	12.1223	6.7546	22.8576
45	A	433	THR	1.7085	1.7868	1.6042
	A	434	THR	7.5244	1.8978	15.0265
	A	435	ALA	7.7753	3.7138	24.0213
	A	436	THR	8.6934	2.5690	16.8594
	A	437	SER	15.8041	3.9341	39.5441
50	A	438	GLY	10.8151	10.8151	0.0000
	A	439	PRO	13.4383	3.2705	26.9955
	A	440	ARG	8.7641	7.5143	9.4782
	A	441	ALA	6.7461	1.8371	26.3821
	A	442	ALA	10.4272	3.2972	38.9468
55	A	443	PRO	1.3762	2.4083	0.0000

	A	444	ALA	9.1593	2.0797	37.4777
	A	445	VAL	0.9848	1.7231	0.0005
	A	446	TYR	3.1461	0.0000	4.7192
	A	447	ALA	0.0289	0.0362	0.0000
	A	448	PHE	0.6153	0.0000	0.9669
	A	449	ALA	3.8692	3.2275	6.4360
	A	450	THR	1.9237	0.4303	3.9148
	A	451	PRO	12.1453	6.5643	19.5866
	A	452	GLU	7.9403	6.9431	8.7381
	A	453	ALA	30.2649	20.0784	71.0111
	A	459	LYS	14.7292	11.5275	17.2907
	A	460	ARG	5.9981	0.0765	9.3819
	A	461	THR	0.1536	0.0000	0.3584
	A	462	LEU	0.0001	0.0002	0.0000
	A	463	ALA	0.0001	0.0001	0.0000
	A	464	CYS	0.0087	0.0130	0.0000
	A	465	LEU	0.0982	0.1233	0.0732
	A	466	ILE	0.0200	0.0000	0.0401
	A	467	GLN	0.8305	0.0002	1.4947
	A	468	ASN	5.9937	1.5627	10.4246
	A	469	PHE	0.0000	0.0000	0.0000
	A	470	MET	7.2629	0.0000	14.5258
	A	471	PRO	1.8851	1.4594	2.4527
	A	472	GLU	7.3364	0.4665	12.8323
	A	473	ASP	5.6153	1.4927	9.7380
	A	474	ILE	3.5567	6.3075	0.8058
	A	475	SER	2.6057	1.5404	4.7363
	A	476	VAL	2.4253	3.4886	1.0077
	A	477	GLN	1.0498	0.0000	1.8897
	A	478	TRP	0.1187	0.2438	0.0687
	A	479	LEU	0.6608	0.0000	1.3216
	A	480	HIS	5.1342	0.7731	8.0417
	A	481	ASN	6.5819	0.8724	12.2914
	A	482	GLU	18.7049	10.4001	25.3487
	A	483	VAL	12.0619	0.7436	27.1528
	A	484	GLN	8.9474	5.5610	11.6565
	A	485	LEU	3.1319	1.3283	4.9354
	A	486	PRO	12.0736	3.3535	23.7005
	A	487	ASP	12.6169	1.7276	23.5062
	A	488	ALA	20.4452	11.0832	57.8933
	A	489	ARG	7.8562	4.5508	9.7450
	A	490	HIS	2.6987	4.4236	1.5488
	A	491	SER	4.4347	1.1905	10.9232
	A	492	THR	5.2960	2.8369	8.5749
	A	493	THR	0.9440	0.7955	1.1420
	A	494	GLN	13.6713	0.9109	23.8796
	A	495	PRO	6.0581	4.4972	8.1393
	A	496	ARG	6.3674	0.9523	9.4618
	A	497	LYS	16.8451	3.4562	27.5561
	A	498	THR	4.5143	6.9964	1.2047
	A	499	ALA	17.0252	11.1864	40.3805
	A	500	GLY	18.8178	18.8178	0.0000
	A	501	SER	5.4365	3.4214	9.4666
	A	502	GLY	2.8894	2.8894	0.0000
	A	503	PHE	3.0581	0.0894	4.7545

	A	504	PHE	0.0656	0.0228	0.0900
	A	505	VAL	0.2424	0.0053	0.5586
	A	506	PHE	0.0016	0.0039	0.0003
	A	507	SER	0.0350	0.0179	0.0692
	A	508	ARG	0.6294	0.6714	0.6054
	A	509	LEU	0.0392	0.0185	0.0599
	A	510	GLU	1.7287	1.2093	2.1442
	A	511	VAL	0.3299	0.5773	0.0000
	A	512	THR	10.6447	1.4856	22.8569
	A	513	ARG	9.5285	0.8196	14.5051
	A	514	ALA	14.8713	4.4288	56.6415
	A	515	GLU	3.0827	1.0010	4.7481
	A	516	TRP	3.3932	0.5950	4.5125
	A	517	GLU	12.8907	5.2405	19.0109
	A	518	ALA	5.1774	0.5587	23.6525
	A	519	LYS	3.0790	0.0000	5.5422
	A	520	ASP	10.4782	3.6427	17.3137
	A	521	GLU	7.1047	0.7149	12.2165
	A	522	PHE	0.0000	0.0000	0.0001
	A	523	ILE	3.5408	0.0000	7.0817
	A	524	CYS	0.0000	0.0000	0.0000
	A	525	ARG	4.6100	0.0000	7.2442
	A	526	ALA	0.0902	0.1128	0.0000
	A	527	VAL	0.0669	0.0002	0.1558
	A	528	HIS	0.1300	0.0054	0.2131
	A	529	GLU	7.9604	2.2867	12.4993
	A	530	ALA	4.2802	4.7817	2.2743
	A	531	ALA	0.7347	0.7875	0.5235
	A	532	SER	15.8770	7.2992	33.0325
	A	533	PRO	12.8146	2.0699	27.1409
	A	534	SER	13.2955	4.9891	29.9083
	A	535	GLN	4.3097	0.0000	7.7574
	A	536	THR	5.4579	3.7045	7.7958
	A	537	VAL	5.1081	1.4055	10.0450
	A	538	GLN	8.2068	4.5359	11.1435
	A	539	ARG	10.8337	1.0576	16.4201
	A	540	ALA	9.1994	1.8430	38.6251
	A	541	VAL	1.0570	1.8498	0.0000
	A	542	SER	8.0549	3.4723	17.2202
	A	543	VAL	18.5723	20.6424	15.8122
	A	2	NAG	16.4353	0.0000	16.4353
	B	336	VAL	10.7710	10.1163	11.6438
	B	337	SER	6.7303	0.9166	18.3577
	B	338	ALA	2.1458	2.6822	0.0000
	B	339	TYR	8.0696	1.1676	11.5206
	B	340	LEU	3.9394	7.4662	0.4127
	B	341	SER	10.1645	1.0695	28.3545
	B	342	ARG	6.0757	3.9259	7.3041
	B	343	PRO	1.0733	1.5124	0.4878
	B	344	SER	7.7643	2.0338	19.2253
	B	345	PRO	1.3185	0.0201	3.0497
	B	346	PHE	4.8258	0.0000	7.5834
	B	347	ASP	3.9197	0.0000	7.8394
	B	348	LEU	1.9999	0.7895	3.2104
	B	349	PHE	4.1817	4.2283	4.1551

	B	350	ILE	7.9930	2.5475	13.4385
	B	351	ARG	12.3730	6.6042	15.6695
	B	352	LYS	15.0045	3.9474	23.8501
	B	353	SER	8.5948	1.6503	22.4838
	B	354	PRO	0.2553	0.1754	0.3617
	B	355	THR	5.9200	1.2321	12.1705
	B	356	ILE	0.1391	0.2781	0.0000
	B	357	THR	5.2617	0.3654	11.7900
	B	358	CYS	0.0000	0.0000	0.0000
	B	359	LEU	3.5340	0.0000	7.0680
	B	360	VAL	0.5390	0.0799	1.1511
	B	361	VAL	3.7224	0.1093	8.5398
	B	362	ASP	1.8094	0.3525	3.2662
	B	363	ALA	20.0439	10.4606	58.3772
	B	364	ALA	15.3707	4.9576	57.0231
	B	365	PRO	9.1152	4.3450	15.4754
	B	366	ALA	18.8285	10.0035	54.1287
	B	367	LYS	14.1725	9.5150	17.8985
	B	368	GLY	19.0630	19.0630	0.0000
	B	369	ALA	13.0115	3.7971	49.8693
	B	370	VAL	1.7523	0.1998	3.8225
	B	371	ASN	10.0509	0.2812	19.8206
	B	372	LEU	3.4036	6.2343	0.5729
	B	373	THR	11.1077	0.8564	24.7761
	B	374	TRP	1.5073	3.6124	0.6652
	B	375	SER	8.3615	0.6614	23.7617
	B	376	ARG	3.0771	1.9562	3.7176
	B	377	ALA	15.1815	11.3744	30.4099
	B	378	SER	11.4636	9.9129	14.5651
	B	379	GLY	16.5804	16.5804	0.0000
	B	380	LYS	13.2366	1.9343	22.2785
	B	381	PRO	15.6715	3.5998	31.7671
	B	382	VAL	7.5283	6.2163	9.2776
	B	383	ASN	11.4020	3.4390	19.3649
	B	384	HIS	17.6888	3.0947	27.4182
	B	385	SER	9.0145	7.7907	11.4622
	B	386	THR	10.6406	1.1756	23.2606
	B	387	ARG	8.8774	6.6756	10.1356
	B	388	LYS	12.6102	1.7918	21.2649
	B	389	GLU	12.4839	8.7255	15.4906
	B	390	ALA	12.8869	2.5604	54.1927
	B	391	ALA	27.0786	21.9964	47.4075
	B	397	LEU	7.6502	6.6415	8.6588
	B	398	THR	5.7838	0.0392	13.4434
	B	399	VAL	0.3391	0.0000	0.7912
	B	400	THR	3.3805	0.0000	7.8879
	B	401	SER	0.7193	0.0000	2.1579
	B	402	THR	3.7007	0.2432	8.3106
	B	403	LEU	0.1106	0.0003	0.2208
	B	404	PRO	8.1540	0.8611	17.8779
	B	405	VAL	1.5566	2.7241	0.0000
	B	406	GLY	7.1791	7.1791	0.0000
	B	407	THR	7.0853	0.8445	15.4063
	B	408	ALA	12.2481	1.5500	55.0403
	B	409	ASP	7.3052	0.7230	13.8873

	B	410	TRP	0.6460	0.0006	0.9042
	B	411	ILE	12.7563	5.8221	19.6905
	B	412	GLU	16.8891	9.7584	22.5936
	B	413	GLY	9.7410	9.7410	0.0000
5	B	414	GLU	2.5752	2.6119	2.5458
	B	415	THR	5.4692	0.0703	12.6676
	B	416	TYR	0.4512	0.0209	0.6663
	B	417	GLN	7.0959	0.0872	12.7029
	B	418	CYS	0.0000	0.0000	0.0000
10	B	419	ALA	5.4563	0.0000	27.2815
	B	420	VAL	0.0843	0.1418	0.0075
	B	421	THR	9.3197	0.3238	31.3142
	B	422	ALA	3.6164	3.0205	6.0000
	B	423	PRO	8.4785	10.2004	6.1826
15	B	424	ALA	8.6226	3.5932	28.7401
	B	425	LEU	11.9869	8.8343	15.1395
	B	426	PRO	17.5822	10.4491	27.0930
	B	427	ARG	17.4020	2.6803	25.8144
	B	428	ALA	9.7570	5.0751	28.4846
20	B	429	LEU	6.0642	0.7211	11.4073
	B	430	MET	16.0818	5.9456	26.2180
	B	431	ARG	8.0744	1.6123	11.7671
	B	432	SER	12.2372	6.6046	23.5024
	B	433	THR	1.4684	1.6247	1.2601
25	B	434	THR	7.3739	1.2286	15.5676
	B	435	ALA	7.8667	3.8619	23.8858
	B	436	THR	8.4287	2.5153	16.3133
	B	437	SER	15.9443	4.0579	39.7171
	B	438	GLY	10.6293	10.6293	0.0000
30	B	439	PRO	13.9484	3.3166	28.1241
	B	440	ARG	8.8462	7.2368	9.7658
	B	441	ALA	6.9507	1.8590	27.3179
	B	442	ALA	10.4125	3.4391	38.3062
	B	443	PRO	1.4008	2.4371	0.0192
35	B	444	ALA	9.0537	2.0618	37.0209
	B	445	VAL	1.0436	1.8263	0.0000
	B	446	TYR	3.2280	0.0004	4.8418
	B	447	ALA	0.0363	0.0454	0.0000
	B	448	PHE	0.6260	0.0000	0.9837
40	B	449	ALA	3.9414	3.2169	6.8396
	B	450	THR	2.0045	0.4174	4.1205
	B	451	PRO	12.0887	6.8483	19.0759
	B	452	GLU	8.1587	7.1306	8.9811
	B	453	ALA	30.2751	20.7889	68.2199
45	B	459	LYS	14.9002	12.1326	17.1143
	B	460	ARG	6.1453	0.0029	9.6552
	B	461	THR	0.1144	0.0006	0.2661
	B	462	LEU	0.0002	0.0003	0.0000
	B	463	ALA	0.0000	0.0000	0.0000
50	B	464	CYS	0.0113	0.0170	0.0000
	B	465	LEU	0.0910	0.0946	0.0874
	B	466	ILE	0.0219	0.0000	0.0437
	B	467	GLN	0.8389	0.0000	1.5100
	B	468	ASN	5.9301	1.4721	10.3881
55	B	469	PHE	0.0000	0.0000	0.0000

	B	470	MET	7.0813	0.0000	14.1626
	B	471	PRO	1.8331	1.3727	2.4469
	B	472	GLU	7.3943	0.5175	12.8958
	B	473	ASP	5.5075	1.5025	9.5124
5	B	474	ILE	3.5810	6.3586	0.8033
	B	475	SER	2.6182	1.5408	4.7731
	B	476	VAL	2.3682	3.3339	1.0806
	B	477	GLN	1.0871	0.0000	1.9567
	B	478	TRP	0.1016	0.2324	0.0492
10	B	479	LEU	0.5440	0.0000	1.0880
	B	480	HIS	5.2031	0.7382	8.1798
	B	481	ASN	6.8401	0.8806	12.7996
	B	482	GLU	19.0404	11.1613	25.3436
	B	483	VAL	11.8885	0.8953	26.5460
15	B	484	GLN	8.9330	5.5624	11.6295
	B	485	LEU	2.9872	1.1924	4.7819
	B	486	PRO	12.4420	3.2393	24.7123
	B	487	ASP	12.6235	1.8226	23.4245
	B	488	ALA	20.9557	11.2245	59.8807
20	B	489	ARG	7.5032	4.6052	9.1591
	B	490	HIS	2.6761	4.4041	1.5240
	B	491	SER	4.3984	1.1740	10.8470
	B	492	THR	5.2933	2.7736	8.6528
	B	493	THR	0.8019	0.6773	0.9680
25	B	494	GLN	13.6817	0.8084	23.9803
	B	495	PRO	5.9741	4.5062	7.9314
	B	496	ARG	6.4874	0.9751	9.6372
	B	497	LYS	16.4562	3.2776	26.9991
	B	498	THR	4.6427	7.1707	1.2720
30	B	499	ALA	17.5008	11.3708	42.0207
	B	500	GLY	18.7401	18.7401	0.0000
	B	501	SER	5.4215	3.4199	9.4248
	B	502	GLY	2.8691	2.8691	0.0000
	B	503	PHE	2.9965	0.0437	4.6838
35	B	504	PHE	0.0651	0.0203	0.0907
	B	505	VAL	0.2042	0.0000	0.4765
	B	506	PHE	0.0052	0.0143	0.0000
	B	507	SER	0.0331	0.0000	0.0993
	B	508	ARG	0.5554	0.6385	0.5080
40	B	509	LEU	0.0476	0.0286	0.0666
	B	510	GLU	1.7117	1.1583	2.1544
	B	511	VAL	0.3510	0.6142	0.0000
	B	512	THR	10.6600	1.5410	22.8185
	B	513	ARG	9.4359	0.8028	14.3691
45	B	514	ALA	15.2935	4.4804	58.5460
	B	515	GLU	2.9658	1.4237	4.1995
	B	516	TRP	3.3612	0.5404	4.4896
	B	517	GLU	12.5876	4.9796	18.6740
	B	518	ALA	4.6347	0.6025	20.7633
50	B	519	LYS	2.7664	0.0000	4.9795
	B	520	ASP	10.6223	3.6037	17.6410
	B	521	GLU	7.3610	0.6603	12.7216
	B	522	PHE	0.0081	0.0000	0.0128
	B	523	ILE	3.5242	0.0007	7.0477
55	B	524	CYS	0.0000	0.0000	0.0000

	B	525	ARG	4.7547	0.0000	7.4716
	B	526	ALA	0.0709	0.0887	0.0000
	B	527	VAL	0.0762	0.0000	0.1777
	B	528	HIS	0.1255	0.0005	0.2088
	B	529	GLU	7.9368	2.2949	12.4503
	B	530	ALA	4.2207	4.6880	2.3517
	B	531	ALA	0.7409	0.8075	0.4746
	B	532	SER	16.1085	7.5394	33.2468
	B	533	PRO	13.1853	2.0824	27.9892
	B	534	SER	13.2835	4.9738	29.9029
	B	535	GLN	4.1001	0.0000	7.3802
	B	536	THR	5.5193	3.5752	8.1115
	B	537	VAL	5.1049	1.4593	9.9656
	B	538	GLN	8.2211	4.4767	11.2166
	B	539	ARG	10.8149	1.1022	16.3650
	B	540	ALA	8.9590	1.8529	37.3835
	B	541	VAL	1.0803	1.8905	0.0000
	B	542	SER	8.4553	4.0882	17.1897
	B	543	VAL	18.5355	20.8533	15.4451
	B	2	NAG	16.5934	0.0000	16.5934

In another embodiment, the solvent accessibilities of the amino acids in PhFc-Cε3/Cε4$_{1-222}$ are indicated in Table 5.

Table 5. IgE-Fc Residue Exposure

```
>>>> Surface plot for:
>>>>   structure file= 1FP5_easy.mtf
>>>>   coordinate set= 1FP5_easy.pdb
```

				total accessible area		
	segid	resid	resname	residue	mainchain	sidechain
	A	336	VAL	64.9492	37.4745	27.4746
	A	337	SER	39.1673	3.9332	35.2340
	A	338	ALA	8.7894	8.7894	0.0000
	A	339	TYR	125.2426	4.9472	120.2955
	A	340	LEU	29.8639	28.5555	1.3085
	A	341	SER	61.1170	4.9569	56.1601
	A	342	ARG	65.4430	15.2049	50.2381
	A	343	PRO	7.4718	5.8928	1.5790
	A	344	SER	46.7157	8.2264	38.4893
	A	345	PRO	8.9624	0.1428	8.8196
	A	346	PHE	54.3420	0.0000	54.3420
	A	347	ASP	31.5363	0.0000	31.5363
	A	348	LEU	7.5406	3.0628	4.4778
	A	349	PHE	47.0594	17.8090	29.2504
	A	350	ILE	65.6199	9.9606	55.6593
	A	351	ARG	137.9028	24.7368	113.1660
	A	352	LYS	142.0125	20.1726	121.8399
	A	353	SER	48.9241	7.6848	41.2393
	A	354	PRO	2.7838	1.3055	1.4783
	A	355	THR	40.4021	4.8060	35.5961
	A	356	ILE	0.7303	0.7288	0.0015
	A	357	THR	38.1965	1.6685	36.5281
	A	358	CYS	0.0000	0.0000	0.0000
	A	359	LEU	57.2918	0.0000	57.2918
	A	360	VAL	1.4811	0.0000	1.4811
	A	361	VAL	26.4275	0.0000	26.4275
	A	362	ASP	1.6559	0.0000	1.6559
	A	363	LEU	119.6712	9.2033	110.4678
	A	364	ALA	78.7333	14.3696	64.3637
	A	365	PRO	79.3853	32.3651	47.0202
	A	366	SER	40.2168	14.0242	26.1926
	A	367	LYS	212.4325	43.2686	169.1639
	A	368	GLY	39.8856	39.8856	0.0000
	A	369	THR	102.7635	12.0075	90.7560
	A	370	VAL	5.8020	1.2971	4.5049
	A	371	ASN	70.8195	0.5930	70.2265
	A	372	LEU	26.6375	25.3607	1.2768
	A	373	THR	63.8640	3.8953	59.9687
	A	374	TRP	19.5203	12.4611	7.0592
	A	375	SER	49.4189	2.7649	46.6540
	A	376	ARG	31.0928	7.7441	23.3486
	A	377	ALA	77.5219	45.8060	31.7159
	A	378	SER	66.6797	40.4771	26.2025
	A	379	GLY	65.8988	65.8988	0.0000
	A	380	LYS	116.4270	8.7936	107.6334

	A	381	PRO	108.8295	14.6070	94.2226
	A	382	VAL	54.2349	26.8569	27.3780
55	A	383	ASN	86.4753	13.4514	73.0239
	A	384	HIS	173.6417	12.7135	160.9282
	A	385	SER	51.7955	28.3694	23.4261
	A	386	THR	72.2038	3.6585	68.5453
	A	387	ARG	97.7388	26.1865	71.5523
5	A	388	LYS	115.4839	6.8986	108.5853
	A	389	GLU	113.2234	35.2996	77.9238
	A	390	GLU	116.4752	6.3676	110.1076
	A	391	LYS	144.4826	24.7116	119.7710
	A	392	GLN	113.9451	7.7214	106.2237
10	A	393	ARG	217.0740	36.0558	181.0182
	A	394	ASN	127.4447	33.3744	94.0703
	A	395	GLY	23.5351	23.5351	0.0000
	A	396	THR	35.9405	2.2916	33.6489
	A	397	LEU	37.3071	0.3897	36.9174
15	A	398	THR	36.6338	0.1084	36.5254
	A	399	VAL	1.0056	0.0005	1.0051
	A	400	THR	22.9397	0.0005	22.9392
	A	401	SER	4.2325	0.0010	4.2315
	A	402	THR	25.0142	0.7905	24.2237
20	A	403	LEU	1.2610	0.0000	1.2610
	A	404	PRO	55.8249	3.3119	52.5130
	A	405	VAL	10.7120	10.7120	0.0000
	A	406	GLY	30.1703	30.1703	0.0000
	A	407	THR	48.6461	5.0988	43.5474
25	A	408	ARG	142.5092	1.0113	141.4979
	A	409	ASP	56.6478	3.0794	53.5684
	A	410	TRP	1.0792	0.0006	1.0786
	A	411	ILE	66.2093	21.0455	45.1638
	A	412	GLU	145.4881	39.5895	105.8986
30	A	413	GLY	38.6895	38.6895	0.0000
	A	414	GLU	22.1923	9.2475	12.9448
	A	415	THR	40.6026	0.2438	40.3588
	A	416	TYR	5.1230	0.0308	5.0922
	A	417	GLN	62.3280	0.4057	61.9222
35	A	418	CYS	0.0000	0.0000	0.0000
	A	419	ARG	103.9206	0.0000	103.9206
	A	420	VAL	2.3852	1.4107	0.9744
	A	421	THR	46.0180	1.1126	44.9053
	A	422	HIS	16.6307	8.9744	7.6562
40	A	423	PRO	63.0244	42.0681	20.9562
	A	424	HIS	126.3997	30.4096	95.9901
	A	425	LEU	73.4692	13.0120	60.4572
	A	426	PRO	136.4835	43.7065	92.7770
	A	427	ARG	174.1798	16.4322	157.7477
45	A	428	ALA	31.7676	12.1334	19.6342
	A	429	LEU	47.6693	3.3487	44.3206
	A	430	MET	81.9649	21.6349	60.3301
	A	431	ARG	102.1664	3.7496	98.4168
	A	432	SER	74.7559	27.6174	47.1385
50	A	433	THR	12.0200	7.4697	4.5502
	A	434	THR	54.0747	7.5188	46.5559
	A	435	LYS	39.4746	13.2184	26.2562

	A	436	THR	54.0546	6.8840	47.1706
	A	437	SER	92.5356	13.8146	78.7209
	A	438	GLY	44.5439	44.5439	0.0000
	A	439	PRO	95.9599	12.1244	83.8355
	A	440	ARG	85.9106	27.8327	58.0779
	A	441	ALA	31.0495	7.8868	23.1627
	A	442	ALA	52.0384	13.4854	38.5529
	A	443	PRO	9.0934	9.0918	0.0015
	A	444	GLU	50.5501	4.8813	45.6687
	A	445	VAL	1.1996	1.1993	0.0004
	A	446	TYR	33.1189	0.0000	33.1189
	A	447	ALA	0.2103	0.2103	0.0000
	A	448	PHE	6.4091	0.0021	6.4070
	A	449	ALA	18.5169	13.0271	5.4898
	A	450	THR	6.8652	1.0920	5.7732
	A	451	PRO	85.0090	26.0777	58.9313
	A	452	GLU	53.5564	21.4659	32.0906
	A	453	TRP	233.7213	21.0784	212.6428
	A	454	PRO	110.0223	22.9884	87.0339
	A	455	GLY	58.2985	58.2985	0.0000
	A	456	SER	83.8465	35.4457	48.4007
	A	457	ARG	204.5646	33.7345	170.8301
	A	458	ASP	74.3533	35.5320	38.8213
	A	459	LYS	90.8795	5.6494	85.2301
	A	460	ARG	39.6337	0.3815	39.2522
	A	461	THR	0.9440	0.0000	0.9440
	A	462	LEU	0.0000	0.0000	0.0000
	A	463	ALA	0.0022	0.0022	0.0000
	A	464	CYS	0.0189	0.0189	0.0000
	A	465	LEU	0.0024	0.0000	0.0024
	A	466	ILE	0.0969	0.0000	0.0969
	A	467	GLN	4.2986	0.0000	4.2986
	A	468	ASN	45.2933	4.2260	41.0673
	A	469	PHE	0.0016	0.0000	0.0016
	A	470	MET	45.6193	0.0006	45.6187
	A	471	PRO	10.5390	4.5735	5.9655
	A	472	GLU	66.1010	1.3044	64.7966
	A	473	ASP	34.3329	6.6650	27.6679
	A	474	ILE	28.1949	24.7847	3.4102
	A	475	SER	15.8011	5.8009	10.0002
	A	476	VAL	17.7598	14.8483	2.9115
	A	477	GLN	8.8153	0.0008	8.8145
	A	478	TRP	1.6124	0.9129	0.6996
	A	479	LEU	3.6886	0.0000	3.6886
	A	480	HIS	49.2343	0.4256	48.8086
	A	481	ASN	60.9710	12.4862	48.4849
	A	482	GLU	173.7820	37.6217	136.1603
	A	483	VAL	89.3318	4.1549	85.1769
	A	484	GLN	79.3073	21.3545	57.9528
	A	485	LEU	27.3587	5.2803	22.0784
	A	486	PRO	88.6492	13.2533	75.3958
	A	487	ASP	99.0020	6.5842	92.4178
	A	488	ALA	91.2923	30.7006	60.5917
	A	489	ARG	85.3735	17.3474	68.0262
	A	490	HIS	27.1818	17.0174	10.1644

	A	491	SER	25.4648	5.3465	20.1183
	A	492	THR	37.6322	11.4738	26.1583
55	A	493	THR	6.2876	3.0406	3.2469
	A	494	GLN	120.0995	2.7999	117.2995
	A	495	PRO	41.3128	17.2964	24.0164
	A	496	ARG	67.3088	3.7186	63.5902
	A	497	LYS	150.2799	14.2135	136.0663
5	A	498	THR	38.1648	34.4749	3.6899
	A	499	LYS	148.5493	8.5618	139.9875
	A	500	GLY	76.9764	76.9764	0.0000
	A	501	SER	35.3537	27.8013	7.5524
	A	502	GLY	8.6018	8.6018	0.0000
10	A	503	PHE	31.7527	1.3561	30.3966
	A	504	PHE	0.8997	0.1297	0.7700
	A	505	VAL	1.3819	0.0043	1.3776
	A	506	PHE	0.0393	0.0393	0.0000
	A	507	SER	0.0697	0.0697	0.0000
15	A	508	ARG	7.6439	2.8043	4.8396
	A	509	LEU	0.3316	0.0344	0.2972
	A	510	GLU	22.5879	7.4305	15.1574
	A	511	VAL	7.0471	7.0471	0.0000
	A	512	THR	80.5746	7.4380	73.1367
20	A	513	ARG	111.1689	3.1148	108.0541
	A	514	ALA	58.1366	5.4416	52.6950
	A	515	GLU	27.2188	0.1935	27.0253
	A	516	TRP	44.3047	2.1698	42.1350
	A	517	GLU	113.2078	31.9303	81.2775
25	A	518	GLN	44.8077	1.3672	43.4405
	A	519	LYS	31.0147	0.0000	31.0147
	A	520	ASP	84.0782	14.7455	69.3327
	A	521	GLU	67.8496	3.1378	64.7117
	A	522	PHE	2.3708	0.0000	2.3708
30	A	523	ILE	19.4152	0.0000	19.4152
	A	524	CYS	0.0000	0.0000	0.0000
	A	525	ARG	53.8480	0.0000	53.8480
	A	526	ALA	0.1543	0.1521	0.0022
	A	527	VAL	0.4091	0.0000	0.4091
35	A	528	HIS	0.9368	0.0000	0.9368
	A	529	GLU	49.8255	6.7170	43.1084
	A	530	ALA	25.3085	22.0423	3.2662
	A	531	ALA	3.8937	3.7960	0.0977
	A	532	SER	93.9367	25.5989	68.3378
40	A	533	PRO	113.4963	7.9201	105.5762
	A	534	SER	69.1432	17.4384	51.7047
	A	535	GLN	39.0154	0.0000	39.0154
	A	536	THR	47.4246	15.9885	31.4361
	A	537	VAL	37.3796	5.2662	32.1134
45	A	538	GLN	80.4137	17.3329	63.0807
	A	539	ARG	114.1401	5.3396	108.8005
	A	540	ALA	46.1789	7.2011	38.9778
	A	541	VAL	7.4375	7.4375	0.0000
	A	542	SER	53.4887	16.3308	37.1580
50	A	543	VAL	143.3700	54.8988	88.4713
	B	336	VAL	63.0733	35.0684	28.0049
	B	337	SER	40.7513	3.7350	37.0163

	B	338	ALA	8.2164	8.2164	0.0000
	B	339	TYR	124.9616	4.9609	120.0006
	B	340	LEU	32.2736	30.2378	2.0358
	B	341	SER	59.0456	4.4001	54.6455
	B	342	ARG	68.6573	15.2123	53.4449
	B	343	PRO	7.5644	6.0344	1.5300
	B	344	SER	46.7394	8.2658	38.4735
	B	345	PRO	8.8647	0.0661	8.7987
	B	346	PHE	52.7081	0.0001	52.7079
	B	347	ASP	32.0935	0.0000	32.0935
	B	348	LEU	14.8371	3.0411	11.7960
	B	349	PHE	49.2963	17.4349	31.8613
	B	350	ILE	66.6755	11.3996	55.2758
	B	351	ARG	138.6156	27.1648	111.4508
	B	352	LYS	141.4297	19.8862	121.5435
	B	353	SER	50.0186	7.0285	42.9901
	B	354	PRO	2.2374	0.7342	1.5032
	B	355	THR	41.7632	5.0415	36.7217
	B	356	ILE	0.7365	0.7350	0.0014
	B	357	THR	38.2632	1.6972	36.5659
	B	358	CYS	0.0000	0.0000	0.0000
	B	359	LEU	56.1126	0.0000	56.1126
	B	360	VAL	1.5816	0.0000	1.5816
	B	361	VAL	25.9197	0.0054	25.9143
	B	362	ASP	1.8960	0.0000	1.8960
	B	363	LEU	118.5662	9.4704	109.0958
	B	364	ALA	77.0955	14.3989	62.6966
	B	365	PRO	85.8755	32.6618	53.2137
	B	366	SER	43.4697	13.7975	29.6721
	B	367	LYS	206.9839	38.4032	168.5807
	B	368	GLY	38.3029	38.3029	0.0000
	B	369	THR	104.4643	11.7881	92.6762
	B	370	VAL	5.3648	1.3354	4.0294
	B	371	ASN	71.8454	0.6766	71.1688
	B	372	LEU	27.2777	25.4561	1.8216
	B	373	THR	63.4130	3.0688	60.3442
	B	374	TRP	21.1747	14.5837	6.5910
	B	375	SER	49.3968	2.8090	46.5877
	B	376	ARG	33.5679	7.8441	25.7238
	B	377	ALA	75.8852	45.5987	30.2865
	B	378	SER	67.8229	40.7526	27.0703
	B	379	GLY	66.3404	66.3404	0.0000
	B	380	LYS	120.5164	9.2949	111.2215
	B	381	PRO	109.6176	14.2385	95.3791
	B	382	VAL	53.1169	25.2918	27.8251
	B	383	ASN	91.8842	12.6656	79.2186
	B	384	HIS	177.7631	13.1140	164.6491
	B	385	SER	54.1445	30.9373	23.2073
	B	386	THR	75.0451	3.9383	71.1068
	B	387	ARG	103.3354	27.2889	76.0466
	B	388	LYS	118.3613	6.6694	111.6919
	B	389	GLU	102.2353	27.4529	74.7824
	B	390	GLU	111.8330	2.2529	109.5801
	B	391	LYS	164.3363	16.4358	147.9005
	B	392	GLN	115.7355	9.9426	105.7929

	B	393	ARG	243.1959	43.7367	199.4592
	B	394	ASN	128.7879	34.6864	94.1016
55	B	395	GLY	24.2780	24.2780	0.0000
	B	396	THR	36.3774	3.2281	33.1493
	B	397	LEU	41.3144	1.2301	40.0844
	B	398	THR	36.2084	0.1877	36.0207
	B	399	VAL	0.9349	0.0000	0.9349
5	B	400	THR	22.7308	0.0000	22.7308
	B	401	SER	4.4619	0.0000	4.4619
	B	402	THR	26.2017	0.7838	25.4179
	B	403	LEU	1.0199	0.0000	1.0199
	B	404	PRO	56.9154	3.8109	53.1046
10	B	405	VAL	12.3109	12.3109	0.0000
	B	406	GLY	29.3614	29.3614	0.0000
	B	407	THR	42.7403	3.8469	38.8934
	B	408	ARG	157.6823	3.1126	154.5697
	B	409	ASP	51.4385	3.0432	48.3953
15	B	410	TRP	9.3345	0.0000	9.3345
	B	411	ILE	95.1467	19.7743	75.3724
	B	412	GLU	125.4698	37.7238	87.7460
	B	413	GLY	18.7812	18.7812	0.0000
	B	414	GLU	22.6140	9.6511	12.9629
20	B	415	THR	39.5185	0.3206	39.1980
	B	416	TYR	5.9881	0.0409	5.9472
	B	417	GLN	62.6966	0.3477	62.3489
	B	418	CYS	0.0000	0.0000	0.0000
	B	419	ARG	102.6084	0.0000	102.6084
25	B	420	VAL	2.7707	1.6846	1.0861
	B	421	THR	46.0095	0.8195	45.1900
	B	422	HIS	16.7868	8.9411	7.8457
	B	423	PRO	62.8378	41.9162	20.9217
	B	424	HIS	125.3588	30.3775	94.9814
30	B	425	LEU	71.5870	12.6261	58.9609
	B	426	PRO	136.6526	45.8124	90.8402
	B	427	ARG	170.2552	16.6453	153.6099
	B	428	ALA	32.0708	12.4769	19.5939
	B	429	LEU	48.8898	2.1566	46.7332
35	B	430	MET	84.2805	22.5773	61.7032
	B	431	ARG	100.5128	3.0888	97.4240
	B	432	SER	75.1133	26.0086	49.1047
	B	433	THR	10.4817	6.7238	3.7580
	B	434	THR	48.7159	5.3780	43.3380
40	B	435	LYS	72.0172	7.7237	64.2934
	B	436	THR	58.8140	9.6274	49.1866
	B	437	SER	83.7729	12.9694	70.8035
	B	438	GLY	44.1275	44.1275	0.0000
	B	439	PRO	98.8394	12.2219	86.6175
45	B	440	ARG	88.9167	29.3709	59.5458
	B	441	ALA	32.3694	7.8101	24.5593
	B	442	ALA	52.2561	13.8471	38.4090
	B	443	PRO	9.1527	9.0687	0.0839
	B	444	GLU	77.6629	1.5591	76.1038
50	B	445	VAL	2.0960	2.0960	0.0000
	B	446	TYR	36.2935	0.0000	36.2935
	B	447	ALA	0.1863	0.1863	0.0000

	B	448	PHE	6.5491	0.0000	6.5491
	B	449	ALA	18.6090	12.5251	6.0838
	B	450	THR	4.4299	1.1588	3.2711
	B	451	PRO	76.6290	22.7457	53.8833
	B	452	GLU	55.5072	22.2581	33.2491
	B	453	TRP	235.9264	21.1124	214.8139
	B	454	PRO	111.4380	22.8008	88.6373
	B	455	GLY	74.9059	74.9059	0.0000
	B	456	SER	92.2118	45.4910	46.7208
	B	457	ARG	219.5241	23.6314	195.8927
	B	458	ASP	71.4157	34.5621	36.8536
	B	459	LYS	95.3227	8.3619	86.9608
	B	460	ARG	40.1231	0.1393	39.9838
	B	461	THR	1.4382	0.0000	1.4382
	B	462	LEU	0.0000	0.0000	0.0000
	B	463	ALA	0.0000	0.0000	0.0000
	B	464	CYS	0.0199	0.0199	0.0000
	B	465	LEU	0.7613	0.4703	0.2910
	B	466	ILE	0.1384	0.0000	0.1384
	B	467	GLN	6.3987	0.0000	6.3987
	B	468	ASN	44.9702	3.7128	41.2575
	B	469	PHE	0.0026	0.0000	0.0026
	B	470	MET	46.3764	0.0005	46.3759
	B	471	PRO	15.0525	5.0794	9.9731
	B	472	GLU	65.5924	1.4428	64.1496
	B	473	ASP	46.5992	6.7495	39.8497
	B	474	ILE	28.5269	25.0290	3.4979
	B	475	SER	15.9668	5.7847	10.1821
	B	476	VAL	17.4473	14.3713	3.0760
	B	477	GLN	9.3877	0.0000	9.3877
	B	478	TRP	1.3921	0.8722	0.5198
	B	479	LEU	4.3690	0.0000	4.3690
	B	480	HIS	54.2843	0.6477	53.6366
	B	481	ASN	58.4959	9.8012	48.6946
	B	482	GLU	167.3206	33.4531	133.8675
	B	483	VAL	89.2539	4.2127	85.0413
	B	484	GLN	76.3506	21.2575	55.0931
	B	485	LEU	25.8432	4.5546	21.2886
	B	486	PRO	85.9602	12.9613	72.9989
	B	487	ASP	101.5779	6.8540	94.7239
	B	488	ALA	89.7437	31.7759	57.9678
	B	489	ARG	83.4391	17.2390	66.2001
	B	490	HIS	27.4157	17.3316	10.0841
	B	491	SER	24.9127	5.0237	19.8890
	B	492	THR	37.6675	11.4176	26.2499
	B	493	THR	5.6950	2.6368	3.0582
	B	494	GLN	117.7065	3.0565	114.6500
	B	495	PRO	40.3432	17.1857	23.1575
	B	496	ARG	70.2823	3.8397	66.4426
	B	497	LYS	150.2087	14.1413	136.0674
	B	498	THR	37.9054	34.1687	3.7367
	B	499	LYS	148.9955	8.7157	140.2798
	B	500	GLY	79.0145	79.0145	0.0000
	B	501	SER	35.5772	28.0187	7.5585
	B	502	GLY	8.7428	8.7428	0.0000

	B	503	PHE	31.0098	0.6811	30.3286
	B	504	PHE	0.8456	0.1156	0.7300
55	B	505	VAL	1.3055	0.0259	1.2796
	B	506	PHE	0.0679	0.0679	0.0000
	B	507	SER	0.1087	0.0000	0.1087
	B	508	ARG	7.6625	2.7772	4.8853
	B	509	LEU	0.2769	0.0638	0.2131
5	B	510	GLU	23.9603	7.2457	16.7146
	B	511	VAL	7.2569	7.2569	0.0000
	B	512	THR	80.3374	7.5753	72.7621
	B	513	ARG	111.7661	3.0775	108.6887
	B	514	ALA	68.3844	10.3023	58.0821
10	B	515	GLU	28.0062	5.9456	22.0606
	B	516	TRP	44.6731	2.2532	42.4200
	B	517	GLU	101.0924	22.5848	78.5077
	B	518	GLN	79.1739	0.0000	79.1739
	B	519	LYS	30.5550	0.0000	30.5550
15	B	520	ASP	81.7324	14.5855	67.1468
	B	521	GLU	51.8306	4.1150	47.7156
	B	522	PHE	1.2433	0.0000	1.2433
	B	523	ILE	27.5515	0.0013	27.5502
	B	524	CYS	0.0000	0.0000	0.0000
20	B	525	ARG	53.0495	0.0000	53.0495
	B	526	ALA	0.0470	0.0470	0.0000
	B	527	VAL	0.5077	0.0000	0.5077
	B	528	HIS	0.8503	0.0026	0.8477
	B	529	GLU	70.9722	6.7364	64.2357
25	B	530	ALA	24.8160	21.6506	3.1654
	B	531	ALA	3.8910	3.8714	0.0196
	B	532	SER	93.3813	26.2679	67.1135
	B	533	PRO	112.7473	7.5061	105.2412
	B	534	SER	69.2111	17.8241	51.3871
30	B	535	GLN	38.1066	0.0000	38.1066
	B	536	THR	43.5047	15.6901	27.8146
	B	537	VAL	37.1147	5.1494	31.9653
	B	538	GLN	75.6644	17.3404	58.3241
	B	539	ARG	106.7137	5.0454	101.6683
35	B	540	ALA	44.2412	8.0048	36.2363
	B	541	VAL	7.5264	7.5264	0.0000
	B	542	SER	52.7855	16.1622	36.6233
	B	543	VAL	145.3042	56.7124	88.5918

Residues that are solvent accessible are important as they represent amino acids that are on the external surface of the protein and, as such, may be involved in binding of a FcR to an antibody and be useful in designing proteins with an enhanced binding activity or in identifying compounds that inhibit such binding. In addition, solvent accessible residues can represent targets for modification to produce a Fc region of an antibody with improved function. Such analysis also identifies residues in the interior, or core, of the proteins in the complex. Such residues can also be targeted to produce proteins with improved functions, such as enhanced stability.

A model of the present invention also provides additional information that is not available from other sources. For example, a model can identify the crystal contacts between crystals and predict the location of the FcR binding domain, including those amino acids that actually form contacts with a FcR. Particularly important regions of the model representing the coordinates of Table 1, Table 2 or Table 3 include, but are not limited to the interdomain groove (i.e., space, gap) between the two Cε3/Cε4-containing chains of the IgE antibody Fc region, the hinge between the Cε3 and Cε4 domains of the Fc region, and a loop involved in FcεRIα protein binding, such as the linker between Cε2 and Cε3, the BC loop of Cε3, the DE loop of Cε3, and the FG loop of Cε3. These sites are described in more detail in the Examples and represent sites to target for drug design and mutein production.

A model of the present invention can also represent a complex that includes a Fc domain of an antibody that binds to a FcεRIα protein with an affinity that is at least equivalent to the affinity of a human IgE antibody Fc-Cε3/Cε4 region for the extracellular domain of any of the following FcεRIα proteins: a human FcεRIα protein, a canine FcεRIα protein, a feline FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein and a rat FcεRIα protein. Such a model can represent a FceRI-binding domain of a human, canine, feline, equine, murine or rat Fc region. Such a model can also represent a Fc region with altered substrate specificity, preferably designed based on a model of the present invention.

The present invention includes a model that represents a Fc domain that binds to a Fc receptor of its respective class. Also included is a model that represents a Fc region

of an antibody designed to bind to a Fc receptor of a class other than the class to which the protein naturally binds. Such classes include IgA, IgD, IgE, IgG, and IgM. Such a model of the present invention can be produced, for example, by incorporating all or any part of the amino acid sequence of the other antibody into a 3-D model substantially representing the coordinates in Table 1, Table 2 or Table 3. Such an embodiment includes any model that specifically incorporates any Ig domains that are placed in an orientation (packing interfaces and bend angles) that is based on the structure predicted by the coordinates in Table 1, Table 2 or Table 3 or a similar structure such that the distance between the two antibody-binding domains (i.e., Cε3 for IgE) ranges from about 10 angstroms to about 25 angstroms or from about 20 angstroms to about 40 angstroms. As such, both open and closed conformations of Fc regions are included in the present invention. In one embodiment, a model of the present invention is a 3-D model of a FcεRIα binding domain other than a human FcεRIα binding domain. Such proteins and models thereof can be designed by homology modeling.

A preferred modified model of the present invention is a model that has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 10 angstrom when superimposed, using backbone atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1, Table 2 or Table 3. Preferably such a model has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 8 angstroms, preferably less than 7 angstroms, preferably less than 6 angstroms, preferably less than 5 angstroms, preferably less than 4 angstroms, preferably less than 3 angstroms, preferably less than 2 angstroms, and preferably less than 1 angstroms, when superimposed, using backbone atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1, Table 2 or Table 3. In this embodiment, such a model represents a Fc region binding to a FcR. The backbone atoms are those atoms that form the backbone, or 3-D folding pattern, of the model. As such, backbone atoms are the base residues of amino acids, i.e., nitrogen, carbon, the alpha carbon and oxygen. Also preferred is a model modification that includes a Fc region having an amino acid sequence that shares at least about 30%, preferably at least about 40%, more preferably

at least about 45%, more preferably at least about 50%, more preferably at least about 60% and even more preferably at least about 80% amino acid sequence homology, with a Fc-Cε3/Cε4 region of a human IgE antibody, as determined using the program ALIGN with default parameters, optimal global alignment of two sequences with no short-cuts. A preferred model of the present invention represents a FcεRIα-binding domain, i.e., a region that binds to a FcεRIα protein.

One embodiment of the present invention is a 3-D model of a human Fc-Cε3/Cε4 region produced by a method that includes the steps of: (a) crystallizing a human Fc-Cε3/Cε4 region, such as, but not limited to a protein having amino acid sequence SEQ ID NO:2; (b) collecting X-ray diffraction data from the crystallized protein; and (c) determining the model from the X-ray diffraction data, preferably in combination with an amino acid sequence of the protein. A complex for crystal formation can be produced using a variety of techniques well known to those skilled in the art. As disclosed herein, a human Fc-Cε3/Cε4 region to be crystallized is preferably produced in recombinant insect cells transformed with a gene encoding such a region, such as a baculovirus genetically engineered to produce the respective protein. The purity of the Fc-Cε3/Cε4 region must be sufficient to permit the production of crystals that can be analyzed by X-ray crystallography to a resolution that permits determination of a 3-D model of the protein. Preferably the resolution is at least about 4.5 angstroms (i.e., 4.4 angstroms or better), more preferably at least about 4 angstroms, more preferably at least about 3.5 angstroms, more preferably at least about 3.25 angstroms, more preferably at least about 3 angstroms, more preferably at least about 2.5 angstroms, more preferably at least about 2.3 angstroms, more preferably at least about 2 angstroms and even more preferably at least about 1.5 angstroms. Methods to obtain such purity levels are well known to those skilled in the art.

As disclosed herein, a preferred method to crystallize a Fc-Cε3/Cε4 region is by vapor distillation. Particularly preferred methods are disclosed in the Examples. It should be appreciated that the present invention also includes other methods known to those skilled in the art by which such a complex can be crystallized.

3-D models of some proteins have been determined; see, for example, Blundell et al., *Protein Crystallography*, Academic Press, London, 1976. However, as discussed herein, elucidation of the crystal structure of a Fc-Cε3/Cε4 region of a human IgE was difficult. In one embodiment, crystal structure determination includes obtaining high-resolution data using synchrotron radiation. Such data can be collected, for example, at the Stanford Synchrotron Source Laboratory, Palo Alto, CA, or the Advanced Photon Source at Argonne National Laboratories, Argonne, IL. Additional locations to collect such data include, but are not limited to, Brookhaven, NY, and Japan. In one embodiment, diffraction data from native and heavy-atom treated crystals provide an initial image of the protein structure which is refined into an electron density map. Details regarding data collection and interpretation are provided in the Examples section.

One embodiment of the present invention is a method to produce a 3-D model of a Fc region that includes positioning amino acid representations (i.e., representing amino acids) of the protein at substantially the coordinates listed in Table 1, Table 2 or Table 3. That is, knowledge of the coordinates of the complex permits one skilled in the art to produce a model of the protein using those coordinates. Such a model, or any model which is essentially represented by a simple coordinate transformation of the coordinates specified in Table 1, Table 2 or Table 3, can be represented in a variety of methods as heretofore disclosed and is included in the present invention.

In another embodiment, a model of the present invention can be refined to obtain an improved model, which is an example of a model modification, also referred to as a modified model. Refining methods can include, but are not limited to, further data collection and analysis; data collection from frozen crystals; introduction of solvent molecules to the structure; clarification of secondary structure; and analyses of crystallized complexes between a FcR and an antibody or inhibitory compound or of crystallized FcRs or antibodies alone. An additional model refinement method includes analyzing a 3-D model to predict amino acid residues that if replaced are likely to yield proteins with at least one improved function, effecting at least one such replacement, determining whether the activity of the modified protein agrees with the prediction, and refining the model as necessary. Methods to determine whether the modification agrees

with prediction include producing the modified protein and performing assays with that modified protein to determine if the protein does indeed exhibit the improved function(s), such as desired activity, stability and solubility properties. Assays to measure such functions are well known in the art; examples of several such assays are disclosed herein.

Another embodiment of the present invention is a modified 3-D model that represents an antibody other than human IgE as represented by the coordinates in Table 1, Table 2 or Table 3. Preferably the amino acid sequence of the protein(s) to be modeled is known. In such a case, the modified model can be produced using the technique of homology modeling, preferably by incorporating (e.g., grafting, overlaying or replacing) all or any portion of the amino acid sequence of the other antibody into the 3-D model representing the coordinates of Table 1, Table 2 or Table 3 to produce the modified model. General techniques for homology modeling, also referred to as molecular replacement, have been disclosed in, for example, Greer, 1990, *Proteins: Structure, Function, and Genetics 7*, 317-334; Havel et al., 1991, *J. Mol. Biol. 217*, 1-7; Schiffer et al., 1990, *Proteins: Structure, Function, and Genetics 8*, 30-43; and Lattman, 1985, *Methods Enzymol 115*, 55-77. However, such technology has not been applied to Fc regions of IgE antibodies since, until the present invention, no 3-D model of any Fc region of IgE was available. Thus, the present invention now allows the solving of the structures of a number of other natural and mutated forms of antibodies.

In one embodiment, a model of a Fc region, such as, but not limited to a Fc-Cε3/Cε4 region, is produced by extracting the 3-D coordinates from a published figure or building a 3-D model with atoms from other domains wherein FcR-binding domains of the antibody are oriented as predicted for a human Fc-Cε3/Cε4$_{222}$ protein. For example, a model of the present invention can be produced by orienting two known FcR-binding domains into a bent confirmation such that the distance between the domains ranges from about 10 to about 25 angstroms or from about 20 to about 40 angstroms. In another example, a model can be produced by orienting the hinge between two Ig domains in a manner similar to that specified by the coordinates in Table 1, Table 2 or Table 3. Such a model is referred to as a model in which the hinge between two Ig

domains, e.g., between Cε3 and Cε4 are oriented in a manner as specified by the structural coordinates listed in Table 1, Table 2 or Table 3. This model can then be used in further molecular replacement methods. Such methods can include the steps of (a) orienting the model by three rotations; and (b) translating the model in one to three directions to produce additional model modifications.

Suitable antibodies for which a 3-D model can be determined using homology modeling include any mammalian antibody such as a protein that binds to a FcR for IgE, IgG, IgM, IgA or IgD antibodies. Preferred antibodies that bind to FcRs include human, canine, feline, equine, murine and rat antibodies. The present invention also includes the use of other Ig domains to produce models of the present invention.

One embodiment of the present invention is a 3-D model of a Fc region of an antibody in which the protein has an improved function compared to an unmodified protein as well as a method to produce such a modified model. Such an improved function includes, but is not limited to, enhanced activity, enhanced stability and enhanced solubility. Such a modified model can be produced by replacing at least one amino acid based on information derived from analyzing the 3-D model representing the coordinates in Table 1, Table 2 or Table 3, such that the replacement leads to a protein with an improved function. As used herein, a replacement refers to an (i.e., one or more) amino acid substitution, insertion, deletion, inversion and/or derivatization (e.g., acetylation, glycosylation, phosphorylation, PEG modification, biotinylation, and covalent attachment of other ligands or other compounds to the protein. In one embodiment, synthetic chemical methods are used to produce either a fragment or the entire protein to, for example, introduce non-natural amino acids or other chemical compounds into the structure of a Fc region. For example, based on a structure of the present invention, one can design synthetic peptides or larger proteins that could be linked to produce an intact protein with FcR binding activity, the structure allowing one to design the start and stop points for these peptides, e.g., at surface accessible loops. In accordance with the present invention, an amino acid that is substituted or inserted can be a natural amino acid or an unnatural amino acid, including a derivitized amino acid.

Methods to identify regions in the protein that, if changed, yield a protein with an improved function are disclosed below.

The present invention includes use of a 3-D model of the present invention to identify a compound that inhibits binding between a FcR and an antibody. The advantages of using a 3-D model to identify inhibitory compounds are multi-fold in that the model depicts the site at which a Fc region of an antibody binds to its FcR, i.e., the antibody-binding domain, also referred to as the antibody binding site, and the FcR-binding domain, also referred to as the FcR binding site. The antibody binding site and the FcR binding site together form an FcR:antibody interaction site. As such, a large number of potential inhibitory compounds can be initially analyzed without having to perform *in vitro* or *in vivo* laboratory studies. As used herein, methods to identify inhibitory compounds include, but are not limited to, designing inhibitory compounds based on the 3-D model of a Fc region, probing such a 3-D model with compounds that are potential inhibitors in order to identify those compounds that are actually inhibitory of the binding of an antibody to its FcR, screening a compound data base using such a 3-D model to identify compounds that inhibit such binding, and combinations thereof. Methods to use 3-D models to design, probe for, or screen for suitable inhibitory compounds are known to those skilled in the art. In particular, there are a number of computer programs that enable such methods. See, for example, PCT Publication No. WO 95/35367, by Wilson et al., published December 28, 1995, which is incorporated by reference herein in its entirety.

An inhibitory compound can be any natural or synthetic compound that inhibits the binding of an antibody to a FcR. Examples include, but are not limited to, inorganic compounds, oligonucleotides, proteins, peptides, antibodies, antibody fragments, mimetics of peptides or antibodies (such as, mimetics of antibody or receptor binding sites), and other organic compounds. Compounds can inhibit binding in either a competitive or non-competitive manner and can either interact at the binding site or allosterically. An inhibitory compound should be capable of physically and structurally associating with a FcR and/or an antibody such that the compound can inhibit binding between the two entitites. As such, an inhibitory compound is preferably small and is of

a structure that effectively prevents or disrupts binding. Inhibitory compounds can be identified in one or multiple steps. For example, a compound initially identified that inhibits binding between an antibody and FcR to some extent can be used as a lead to design, probe or screen for a compound with improved characteristics, such as greater efficacy, safety, solubility, etc. A preferred inhibitory compound is a compound that is efficacious when administered to an animal in an amount that results in a serum concentration of from about 1 nanomolar (nM) to 100 micromolar (uM), with a concentration of from about 10 nM to 10 uM being more preferred.

One embodiment of the present invention is a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein. Such a method includes the step of using a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 2 or Table 3 to identify such a compound. Included in the present invention are inhibitory compounds that interact directly with the IgE binding domain or the receptor binding domain of the IgE antibody as well as compounds that interact indirectly with such structures. Preferably a compound interacts with at least one of the following regions: a FcεRIα binding domain, an interdomain groove between the two Cε3/Cε4 domains of the antibody Fc region, a hinge between Cε3 and Cε4 domains of the antibody Fc region, and a region of a Cε3 or Cε4 domain, the relative position of which changes by greater than 1 angstrom between closed and receptor-bound Fc-Cε3/Cε4 conformations. It is to be noted that many residues in the Cε3 domains are significantly closer to the Cε4 domains in the closed form of the IgE as compared to the open form. While not being bound by theory, it is believed that molecules that could interact with Cε3 residues and Cε4 residues at the same time but only in the closed form of the IgE, would be potential inhibitors. Regions to target include a set of residues in the two domains whose relative distances change significantly (i.e., by more than 1 angstrom) in comparison of the receptor-bound and closed IgE conformations. Preferably the distance between the two Cε3 domains of the closed conformation of the Fc-Cε3/Cε4 region ranges from about 10 to about 25 angstroms, more preferably from about 10 and 15 angstroms, and even more preferably about 13 angstroms. In a preferred embodiment, an inhibitory compound reacts with at

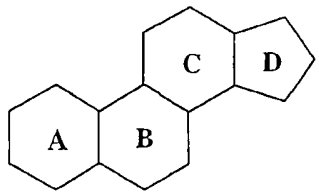
least one of the following regions: a linker between Cε2 and Cε3 (amino acids 4, 7, 8, 9, 10 and 11 of SEQ ID NO:2); a BC loop of Cε3 (amino acids 37, 38 and 39 of SEQ ID NO:2; a DE loop of Cε3 (amino acids 68, 69, and 70 of SEQ ID NO:2); a FG loop of Cε3 (amino acids 99, 100, 101 and 102 of SEQ ID NO:2); a loop or strand defining (i.e., abutting, forming) the interdomain groove; a AB helix of Cε3 (amino acid 20, 21, 22, 23 and 24 of SEQ ID NO:2) which is thought to regulate the full conformational flexibility of the IgE-Fc region; and a region lying above said AB helix of Cε3, i.e., the region constituting the hinge and including amino acids 17, 18 and 19 (after strand A), amino acids 29, 30 and 31 (after strand B), and amino acids 109, 110 and 111 (after strand G) of SEQ ID NO:2. Particularly preferred amino acids with which to have an inhibitory compound interact include: (a) a residue at position 4, 7, 8, 9, 10, 11, 17, 18, 19, 20, 21, 22, 23, 24, 29, 30, 31, 37, 38, 39, 68, 69, 70, 99, 100, 101, 102, 109, 110, or 111 of SEQ ID NO:2; and (b) a surface residue within about 10 angstroms of any of said residues of (a). Even more preferred residues include: (a) a residue at position 4, 7, 8, 9, 10, 11, 37, 38, 39, 68, 69, 70, 99, 100, 101, or 102 of SEQ ID NO:2; (b) a residue in a region of a Cε3 or Cε4 domain, the relative position of which changes by greater than 1 angstrom between closed and receptor-bound Fc-Cε3/Cε4 conformations; and (c) a surface residue within about 10 angstroms of any of said residues of (a) or (b). Also preferred are additional residues identified in the Examples as being in at least one of the above cited regions. One preferred embodiment is a compound that inhibits the ability of an IgE antibody to convert from a closed conformation into a receptor-bound or open conformation. It is to be noted that the ability to identify such key regions and residues is only possible in view of a model of the present invention. In one embodiment, an inhibitory compound of the present invention is a peptide corresponding to at least a portion of any of the identified regions or a derivative thereof, such as a peptide mimetic or other compound that mimics that peptide.

One embodiment of a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein includes the steps of: (a) generating a model substantially representing the atomic coordinates listed in Table 1, Table 2 or Table 3 or of the binding domains thereof, on a computer screen; (b) generating the

spacial structure of a compound to be tested; and (c) testing to determine if the compound interacts with said FcR binding domain, wherein such an interaction indicates that the compound is capable of inhibiting the binding of an IgE antibody to a FcεRIα protein. In a preferred embodiment, step (a) includes the step of identifying one or more amino acid(s) in the FcR binding domain of the model that interact directly with the FcR. Preferably a compound to be tested will interact directly with one or more of those amino acid(s). Preferred amino acids with which an inhibitory compound should interact are disclosed herein.

The present invention also includes inhibitory compounds isolated in accordance with the methods disclosed herein. Methods to produce such compounds in quantities sufficient for use, for example, as protective agents (e.g., preventatives or therapeutics) are known to those skilled in the art. It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of any suitable Fc regions (i.e., model modifications) and to identify compounds that inhibit the binding of antibodies to such Fc regions.

A preferred inhibitory compound of the present invention, or lead that can be used to produce a more efficacious inhibitory compound, is a saturated tetracyclic hydrocarbon perhydrocyclopentanophenanthrene or a derivative thereof. Such a compound can include a structure having the following formula:



It is to be understood that such a compound can have any number of "R" groups, even though they are not indicated in the formula. Examples of saturated tetracyclic hydrocarbon perhydrocyclopentanophenanthrenes include, but are not limited to, isoprenoids, terpenes, bile acids, detergents (such as CHAPS and CHAPSO) cholestanes, cholic acids, cholesterols, androgens, estrogens, and other steroids. A preferred inhibitory compound, or compound to use as a lead to design a more efficacious

compound is 3-[3-(cholamidopropyl) dimethylammonio]-1-propane-sulfonate (CHAPS) or a compound having a similar ring structure. The interaction of CHAPS with amino acids in the FcεRIα protein and Fc-Cε3/Cε4 region is described in further detail in 60/189,853, *ibid.*

In one embodiment, an inhibitory compound of the present invention is a bivalent, or other multivalent, compound that interacts with the two Cε3/Cε4 domains with high affinity or a compound that is sufficiently large to bind the interdomain groove, such as, but not limited to, macromolecules such as *in vitro* selected peptides, peptoids, nucleic acids, similar molecules, mimetopes thereof.

The present invention also includes use of a 3-D model of the present invention to rationally design and construct modified forms of Fc regions of antibodies, and particularly of IgE antibodies, that have one or more improved functions, such as, but not limited to, increased activity, increased stability and increased solubility compared to an unmodified Fc region of an IgE antibody. Muteins of the present invention include full-length proteins as well as fragments (i.e., truncated versions) of such proteins.

One embodiment of the present invention is a Fc region that comprises a mutein that binds to a Fc binding domain of a FcR. Such a mutein has an improved function compared to a protein comprising SEQ ID NO:2. Examples of such an improved function include, but are not limited to, increased stability, increased affinity for an FcR, altered substrate specificity, and increased solubility. Such a mutein can be produced by a method that includes the steps of: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 2 or Table 3 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect the improved function of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having the improved function. Knowledge of the coordinates allows one to target specific residues, e.g. in the hydrophobic core or on the surface, to generate an accessible set of variants that can then be selected for a particular property, e.g. high stability, high affinity, altered substrate specificity, or other desirable properties (i.e., improved functions). Without the coordinates, one would have to analyze an extraordinarily large number of variants, e.g., on the order of ~10^{11}

possibilities. The structure, in contrast, allows one to pick the most relevant residues for selecting a desired property by, for example, phage display or other methods. In a preferred embodiment, replacement of one or more amino acids does not substantially disrupt the 3-D structure of the protein; i.e., the modified protein, or mutein, is still capable of binding to the FcR. A preferred mutein is a Fc domain of an IgE antibody that binds to a FcεRIα protein, although the invention also covers muteins binding to other classes of FcRs.

In one embodiment, a mutein of the present invention has increased stability compared to its unmodified counterpart. As used herein, increased stability refers to the ability of a mutein to be more resistant, for example, to higher or lower temperature, to more acidic or basic pH, to higher or lower salt concentrations, to oxidation and/or reduction, to deamidation, to other forms of chemical degradation and to proteolytic degradation compared to an unmodified Fc region. Increased stability can also refer to the ability of a mutein of the present invention to be stable for a longer period of time either during storage (i.e., to have a longer shelf life) or during use (i.e., to have a longer half-life under reaction conditions) than does an unmodified protein. Muteins of the present invention can also exhibit a decreased entropy of unfolding, thereby stabilizing the proteins. Increased stability can be measured using a variety of methods known to those skilled in the art; examples include, but are not limited to, determination of melting temperature, thermal denaturation, pressure denaturation, enthalpy of unfolding, free energy of the protein, or stability in the presence of a chaotropic agents such as urea, guanidinium chloride, guanidinium thiocyanate, etc. A preferred mutein of the present invention has a melting temperature substantially higher than that of an unmodified Fc region. Preferably the melting temperature of a mutein is at least about 1°C higher, and more preferably at least about 10°C higher than the melting temperature of the corresponding unmodified protein. Also preferred is a mutein having binding activity over a pH range that is at least about 1 pH unit higher and/or lower than the active pH range of the corresponding unmodified protein.

Another embodiment of the present invention is a mutein that exhibits increased affinity for a FcR compared to its unmodified counterpart. As used herein, a mutein

having increased affinity is a Fc region that exhibits a higher affinity constant (K_A) or lower dissociation constant (K_D) than its unmodified counterpart. Such a higher affinity constant can be achieved by increasing the association rate (k_a) between the mutein and the FcR and/or decreasing the dissociation rate (k_d) between the mutein and the FcR . A preferred mutein of the present invention has a K_A for a FcR of at least about 3×10^9 liters/mole (M^{-1}), which is equivalent to a K_D of less than or equal to about 3.3×10^{-10} moles/liter (M). More preferred is a mutein having a K_A for a FcR of at least about 2×10^{10} M^{-1}, and even more preferably of at least about 1×10^{11} M^{-1}. Also preferred is a mutein having a k_a for a FcR of at least about 1×10^5 liters/mole-second as well as a mutein having a k_d for a FcR of less than or equal to 3×10^{-5}/second. More preferred is a mutein having a k_a for a FcR of at least about 3×10^5 liters/mole-second, and even more preferably of 1×10^6 liters/mole-second. Also preferred are muteins having a k_d for a FcR of less than or equal to 1×10^{-5}/second or even more preferably less than or equal to 3×10^{-4}/second. A preferred FcR is FcεRIα. Methods to measure such binding constants is well known to those skilled in the art; see, for example, Cook et al., 1997, *ibid.*, which reports the following values for the binding of human FcεRIα protein to human IgE: k_{a1} of 3.5 ($\pm$0.9) x 10^5 $M^{-1}s^{-1}$; k_{a2} of 8.6 ($\pm$3.5) x 10^4 $M^{-1}s^{-1}$; k_{d1} of 1.2 ($\pm$0.1) x 10^{-2} s^{-1}; k_{d2} of 3.2 ($\pm$0.8) X 10^{-5} s^{-1}; K_{A1} of 2.0 X10^7 M^{-1}; K_{A2} of 2.9 X10^9 M^{-1}.

Another embodiment of the present invention is a mutein that exhibits altered substrate specificity compared to its unmodified counterpart. A mutein exhibiting altered substrate specificity is a mutein that binds with increased affinity to a FcR for an antibody class or antibody species of a different type than that normally bound by its unmodified counterpart. In one embodiment, a mutein of a human Fc-Cε3/Cε4 region with altered substrate specificity is a Fc region that binds with increased affinity to a receptor that binds to an IgE antibody of another mammal, such as, but not limited to, a canine, feline, equine, murine, or rat IgE antibody. In another embodiment, a mutein of a human Fc-Cε3/Cε4 region with altered substrate specificity is a Fc region that binds with increased affinity to a Fc receptor for an antibody of another class, such as IgG, IgM, IgA, or IgD, with IgG being preferred. Such a mutein can also show altered species

substrate specificity. Methods to determine whether a mutein exhibits altered substrate specificity are well known to those skilled in the art.

Yet another embodiment of the present invention is a mutein that exhibits increased solubility compared to its unmodified counterpart. Such a protein is less likely to form aggregates. Methods to determine whether a mutein exhibits increased solubility are well known to those skilled in the art.

As disclosed herein, the 3-D model substantially representing the coordinates in Table 1, Table 2 or Table 3 is advantageous in determining strategies for producing muteins having an improved function, e.g., for identifying targets to modify in order to obtain muteins having improved functions. Examples of targets include, but are not limited to, those regions of the Fc-Cε3/Cε4 region that directly or indirectly interact with a FcεRIα protein.

In accordance with the present invention, a mutein having an improved function can be produced by a method that includes replacing at least one amino acid based on information derived from analyzing a 3-D model of the present invention to produce the mutein having the improved function. Knowledge of the structure of the human Fc-Cε3/Cε4 region, for example, permits the rational design and construction of modified forms of the protein by permitting the prediction and production of substitutions, insertions, deletions, inversions and/or derivatizations that effect an improved function. That is, analysis of 3-D models of the present invention provide information as to which amino acid residues are important and, as such, which amino acids can be changed without harming the protein. In making amino acid replacements, it is preferred to use amino acid replacements that have similar numbers of atoms and that allow conservation of salt bridges, hydrophobic interactions and hydrogen bonds unless the goal is to purposefully change such interactions. The 3-D structure of the human Fc-Cε3/Cε4 region suggests that large deletions may not be desirable, particularly due to the relation between the various domains of the protein and the observation that most of the structure is well ordered in the crystal.

It is to be appreciated that although one amino acid replacement capable of improving the function of a protein can substantially improve that function, more than

one amino acid replacement can result in cumulative changes depending on the number and location of the replacements. For example, although one amino acid replacement capable of substantially increasing the stability of a protein can increase the melting temperature of that modified protein by about 1°C, about 5 to about 6 replacements may increase the melting temperature of the resultant protein by about 10°C.

In accordance with the present invention, the 3-D model of the Fc region has been analyzed, using techniques known to those skilled in the art, to determine the accessibility of the amino acids represented within the model to solvent. Such information is provided in, for example, Table 4 or Table 5.

A number of methods can be used to produce muteins of the present invention. One method includes the steps of: (a) analyzing a 3-D model substantially representing the coordinates specified in Table 1, Table 2 or Table 3 to identify at least one amino acid of the modeled protein which if replaced by a specified amino acid would effect an improved function; and (b) replacing the identified amino acid(s) to produce a mutein having that improved function. In one embodiment, a method to produce a mutein includes the steps of (a) comparing a key region of a model of a human Fc-Cε3/Cε4 region with the amino acid sequence of a Fc region having an improved function compared to the unmodified Fc-Cε3/Cε4 region in order to identify at least one amino acid segment of the Fc region with the improved function that if incorporated into the Fc-Cε3/Cε4 region represented by the model would give the Fc-Cε3/Cε4 region the improved function; and (b) incorporating the segment into the Fc-Cε3/Cε4 region, thereby providing a mutein with the improved function. In another embodiment, a method to produce a protein includes the steps of: (a) using a model representing a human Fc-Cε3/Cε4 region to identify a 3-D arrangement of residues that can be randomized by mutagenesis to allow the construction of a library of molecules from which a improved function can be selected; and (b) identifying at least one member of the mutagenized library having the improved function. In one example, a mutein is produced by a method that includes the steps of: (a) effecting random mutagenesis of nucleic acid molecules encoding a target of a Fc-Cε3/Cε4 region as identified by analyzing a model of that protein, such as an FcR binding domain; (b) cloning such

mutagenized nucleic acid molecules into a phage display library, wherein said phage display library expresses the target; and (c) identifying at least one member of the library that expresses a target with an improved function, such as an FcR binding domain exhibiting increased affinity for an FcR. As stated above, the model allows the use of this technique in a straightforward manner that could not be accomplished in the absence of the model. It is to be also noted that these methods can also be used with other models of the present invention to produce muteins of the present invention.

The present invention includes a number of methods, based on analysis of a 3-D model of the present invention, to replace (i.e., add, delete, substitute, invert, derivatize) at least one amino acid residue in the protein represented by the model in order to produce a mutein of the present invention. Such methods include, but are not limited to: (a) replacing at least one amino acid in at least one non-constrained loop; (b) joining an amino-terminal amino acid residue to a carboxyl-terminal amino acid residue; (c) replacing at least one amino acid site with an amino acid suitable for derivatization; (d) replacing at least one pair of amino acids of the protein with a cysteine pair to enable the formation of a disulfide bond that stabilizes the protein; (e) replacing at least one amino acid in the FcεRIα binding domain in order to increase the affinity between an IgE Fc region and the corresponding FcR; (f) replacing at least one amino acid of the protein with an amino acid such that the replacement decreases the entropy of unfolding of the protein; (g) replacing at least one asparagine or glutamine of the protein with an amino acid that is less susceptible to deamidation than is the amino acid to be replaced; (h) replacing at least one methionine, histidine or tryptophan with an amino acid that is less susceptible to an oxidation or reduction reaction than is the amino acid to be replaced; (i) replacing at least one arginine of the protein with an amino acid that is less susceptible to dicarbonyl compound modification than is the amino acid to be replaced; (j) replacing at least one amino acid of the protein susceptible to reaction with a reducing sugar sufficient to reduce protein function with an amino acid less susceptible to that reaction; (k) replacing at least one amino acid of the protein with an amino acid capable of increasing the stability of the inner core of the protein; (l) replacing at least one amino acid of the protein with at least one N-linked glycosylation site; (m) replacing at least

one N-linked glycosylation site of the protein with at least one amino acid that does not comprise an N-linked glycosylation site; and (n) replacing at least one amino acid of the protein with an amino acid that reduces aggregation of the protein. Muteins of the present invention can be produced using methods and rationales similar to those disclosed in PCT WO 00/26246, *ibid.*; such methods, which are incorporated herein by reference in their entirety, can be applied to Fc-Cε3/Cε4 muteins of the present invention.

Amino acid replacements can be carried out using recombinant DNA techniques known to those skilled in the art, including site-directed mutagenesis (e.g., oligonucleotide mutagenesis, random mutagenesis, polymerase chain reaction (PCR)-aided mutagenesis, gapped-circle site-directed mutagenesis) or chemical synthetic methods of a nucleic acid molecule encoding the desired protein, such as, but not limited to a human FcεRIα protein, followed by expression of the mutated gene in a suitable expression system, preferably an insect, mammalian, bacterial, yeast, insect, or mammalian expression system. See, for example, Sambrook et al., *ibid.*

It is to be appreciated that muteins of the present invention can include amino acids which are not modified because they would negatively impact the function of the protein. Such amino acids can be identified using a 3-D model of the present invention.

It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of and make modifications to any suitable FcRs or other Ig domain-containing proteins to produce muteins having a desired function.

Antibody muteins have a variety of uses, including but not limited to, diagnostic and therapeutic uses. For example, muteins could be used to image cells that express an antibody receptor protein, such as NMR-specific labeling for *in vivo* imaging to detect, for example, mast cell cancers, asthma, and other pathologies, or to treat cancers that express an antibody receptor protein using, for example, radioimmune therapy of derivatized IgE. Muteins could also be used for monitoring FcR expression in atopic individuals (e.g. with a tag for one-step FACS analysis) or for monitoring IgE in atopic individuals. Muteins could also be used as inhibitors or as toxin-IgE-Fc fusion proteins

to target FcR-expressing cells to kill them (e.g. in mast cell tumors or severe allergy). Also muteins that affect the low affinity affinity IgE-receptor (FceRII) binding but not FceRI binding could be designed or selected.

The present invention also includes nucleic acid molecules that encode muteins of the present invention as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Methods to produce such proteins are also disclosed herein.

The present invention also includes the following novel structures as identified by a 3-D model of the present invention. Preferred structures exhibiting direct interaction between IgE and FcεRIα include a FcεRIα binding domain, an interdomain groove between the two Cε3/Cε4 domains of said antibody Fc region, a hinge between Cε3 and Cε4 domains of said antibody Fc region, and a region of a Cε3 or Cε4 domain, the relative position of which changes by greater than 1 angstrom between closed and receptor-bound Fc-Cε3/Cε4 conformations. Preferred compositions include a linker between Cε2 and Cε3, a BC loop of Cε3, a DE loop of Cε3, and a FG loop of Cε3, a loop or strand defining the interdomain groove, a AB helix of Cε3 and, a region lying above said AB helix of Cε3. The present invention also includes nucleic acid molecules to encode such compositions.

The present invention also includes an isolated Fc-Cε3/Cε4 protein selected from the group consisting of: (a) a protein consisting of SEQ ID NO:2; and (b) an isolated protein that is structurally homologous to a protein of (a), wherein said protein of (b) binds to a FcεRIα protein. Also included in the present invention is such a protein produced in insect cells. In one embodiment the Fc-Cε3/Cε4 protein a human Fc-Cε3/Cε4 protein, a canine Fc-Cε3/Cε4 protein, a feline Fc-Cε3/Cε4 protein, an equine Fc-Cε3/Cε4 protein, a murine Fc-Cε3/Cε4 protein, or a rat Fc-Cε3/Cε4 protein. The present invention also includes nucleic acid molecules that encode such proteins, as well as recombinant molecules, recombinant cells and recombinant viruses that include such nucleic acid molecules. Also included are methods to produce such proteins using such nucleic acid molecules, recombinant molecules, recombinant viruses and recombinant cells.

The present invention also includes isolated nucleic acid molecules encoding proteins of the present invention, including, but not limited to, unmodified proteins, novel structures within such proteins, and muteins. As used herein, an isolated nucleic acid molecule encoding a protein is a nucleic acid molecule that has been removed from its natural milieu. As such, "isolated" does not reflect the extent to which the nucleic acid molecule has been purified. An isolated nucleic acid molecule can be DNA, RNA, or derivatives of either DNA or RNA.

A nucleic acid molecule encoding a mutein of the present invention can be produced by mutation of parental protein genes (e.g., unmodified or previously modified protein-encoding genes, or portions thereof) using recombinant DNA techniques heretofore disclosed or by chemical synthesis. Resultant mutein nucleic acid molecules can be amplified using recombinant DNA techniques known to those skilled in the art, such as PCR amplification or cloning (see, for example, Sambrook et al., *ibid.*), or by chemical synthesis. A mutein can also be produced by chemical modification of a protein expressed by a nucleic acid molecule encoding an unmodified protein or mutein-encoding gene.

Proteins of the present invention can be produced in a variety of ways, including production and recovery of recombinant proteins and chemical synthesis. In one embodiment, a protein of the present invention is produced by culturing a cell capable of expressing the protein under conditions effective to produce the protein, and recovering the protein. A preferred cell to culture is a recombinant cell that is capable of expressing the protein, the recombinant cell being produced by transforming a host cell with one or more nucleic acid molecules of the present invention. Transformation of a nucleic acid molecule into a host cell can be accomplished by any method by which a nucleic acid molecule can be inserted into a cell. Transformation techniques include, but are not limited to, transfection, electroporation, microinjection, lipofection, adsorption, and protoplast fusion. A recombinant cell may remain unicellular or may grow into a tissue, organ or a multicellular organism. Transformed nucleic acid molecules of the present invention can remain extrachromosomal or can integrate into one or more sites within a chromosome of a host cell in such a manner that their ability to be expressed is retained.

Suitable host cells to transform include any cell that can be transformed. Host cells can be either untransformed cells or cells that are already transformed with at least one nucleic acid molecule. Host cells of the present invention can be endogenously (i.e., naturally) capable of producing a protein of the present invention, but such cells are not preferred. Host cells of the present invention can be any cell that when transformed with a nucleic acid molecule of the present invention are capable of producing a protein of the present invention, including bacterial, yeast, other fungal, insect, animal, and plant cells. Preferred host cells include bacterial, yeast, insect and mammalian cells, and more preferred host cells include *Escherichia*, *Bacillus*, *Saccharomyces, Pichia*, *Trichoplusia*, *Spodoptera* and mammalian cells. Particularly preferred host cells are *Trichoplusia ni* cells and *Spodoptera frugiperda* cells with *T. ni* cells being particularly preferred.

A recombinant cell is preferably produced by transforming a host cell with a recombinant molecule comprising a nucleic acid molecule of the present invention operatively linked to an expression vector containing one or more transcription control sequences. The phrase operatively linked refers to insertion of a nucleic acid molecule into an expression vector in a manner such that the molecule is able to be expressed when transformed into a host cell. As used herein, an expression vector is a DNA or RNA vector that is capable of transforming a host cell, of replicating within the host cell, and of effecting expression of a specified nucleic acid molecule. Expression vectors can be either prokaryotic or eukaryotic, and are typically viruses or plasmids. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including in bacterial, yeast, other fungal, insect, animal, and plant cells. Preferred expression vectors of the present invention can direct gene expression in bacterial, yeast, insect and mammalian cells.

Nucleic acid molecules of the present invention can be operatively linked to expression vectors containing regulatory control sequences such as promoters, operators, repressors, enhancers, termination sequences, origins of replication, and other regulatory control sequences that are compatible with the host cell and that control the expression of the nucleic acid molecules. In particular, recombinant molecules of the present invention include transcription control sequences. Transcription control sequences are

sequences which control the initiation, elongation, and termination of transcription. Particularly important transcription control sequences are those which control transcription initiation, such as promoter, enhancer, operator and repressor sequences. Suitable transcription control sequences include any transcription control sequence that can function in at least one of the recombinant cells of the present invention. A variety of such transcription control sequences are known to those skilled in the art. Preferred transcription control sequences include those which function in bacterial, yeast, insect and mammalian cells.

It may be appreciated by one skilled in the art that use of recombinant DNA technologies can improve expression of transformed nucleic acid molecules by manipulating, for example, the number of copies of the nucleic acid molecules within a host cell, the efficiency with which those nucleic acid molecules are transcribed, the efficiency with which the resultant transcripts are translated, and the efficiency of post-translational modifications. Recombinant techniques useful for increasing the expression of nucleic acid molecules of the present invention include, but are not limited to, operatively linking nucleic acid molecules to high-copy number plasmids, integration of the nucleic acid molecules into one or more host cell chromosomes, addition of vector stability sequences to plasmids, substitutions or modifications of transcription control signals (e.g., promoters, operators, enhancers), substitutions or modifications of translational control signals (e.g., ribosome binding sites, Shine-Dalgarno sequences), modification of nucleic acid molecules of the present invention to correspond to the codon usage of the host cell, deletion of sequences that destabilize transcripts, and use of control signals that temporally separate recombinant cell growth from recombinant protein production during fermentation. The activity of an expressed recombinant protein of the present invention may be improved by fragmenting, modifying, or derivatizing nucleic acid molecules encoding such a protein.

In accordance with the present invention, recombinant cells can be used to produce proteins by culturing such cells under conditions effective to produce such a protein, and recovering the protein. Effective conditions to produce a protein include, but are not limited to, appropriate media, bioreactor, temperature, pH and oxygen conditions

that permit protein production. An appropriate medium refers to any medium in which a cell of the present invention, when cultured, is capable of producing the protein. An effective medium is typically an aqueous medium comprising assimilable carbohydrate, nitrogen and phosphate sources, as well as appropriate salts, minerals, metals and other nutrients, such as vitamins. The medium may comprise complex nutrients or may be a defined minimal medium. Cells of the present invention can be cultured in conventional fermentation bioreactors, which include, but are not limited to, batch, fed-batch, cell recycle, and continuous fermentors. Culturing can also be conducted in shake flasks, test tubes, microtiter dishes, and petri plates. Culturing is carried out at a temperature, pH and oxygen content appropriate for the recombinant cell. Such culturing conditions are well within the expertise of one of ordinary skill in the art.

Depending on the vector and host system used for production, resultant proteins may either remain within the recombinant cell; be secreted into the fermentation medium; be secreted into a space between two cellular membranes, such as the periplasmic space in *E. coli*; or be retained on the outer surface of a cell or viral membrane. The phrase "recovering the protein" refers simply to collecting the whole fermentation medium containing the protein and need not imply additional steps of separation or purification. Proteins of the present invention can be purified using a variety of standard protein purification techniques, such as, but not limited to, affinity chromatography, ion exchange chromatography, filtration, electrophoresis, hydrophobic interaction chromatography, gel filtration chromatography, reverse phase chromatography, chromatofocusing and differential solubilization.

The present invention also includes isolated (i.e., removed from their natural milieu) antibodies that selectively bind to a Fc region of the present invention. As used herein, the term "selectively binds to" refers to the ability of antibodies of the present invention to preferentially bind to an Fc region of the present invention. Binding can be measured using a variety of methods standard in the art including enzyme immunoassays (e.g., ELISA), immunoblot assays, etc.; see, for example, Sambrook et al., *ibid.* Isolated antibodies of the present invention can include antibodies in a bodily fluid (such as, but not limited to, serum), or antibodies that have been purified to varying degrees.

Antibodies of the present invention can be polyclonal or monoclonal. Functional equivalents of such antibodies, such as antibody fragments and genetically-engineered antibodies (including single chain antibodies or chimeric antibodies that can bind to more than one epitope) are also included in the present invention. Antibodies can be produced using methods known to those skilled in the art. A preferred method to produce antibodies of the present invention includes (a) administering to an animal an effective amount of a protein of the present invention to produce the antibodies and (b) recovering the antibodies. In another method, antibodies of the present invention are produced recombinantly using techniques as heretofore disclosed to produce proteins of the present invention. Antibodies raised against defined proteins can be advantageous because such antibodies are not substantially contaminated with antibodies against other substances that might otherwise cause interference in a diagnostic assay or side effects if used in a therapeutic composition.

Antibodies of the present invention have a variety of potential uses that are within the scope of the present invention. Examples of such uses are disclosed in WO 98/27208, *ibid.*, see, for example, page 24; such uses are incorporated by reference herein in their entireties.

A Fc region of the present invention can include chimeric molecules comprising at least a portion of a Fc region that binds to an antibody and a second molecule that enables the chimeric molecule to be bound to a substrate in such a manner that the antibody receptor portion binds to the antibody in at least as effective a manner as a Fc region that is not bound to a substrate. An example of a suitable second molecule includes a portion of an immunoglobulin molecule or another ligand that has a suitable binding partner that can be immobilized on a substrate, e.g., biotin and avidin, or a metal-binding protein and a metal (e.g., His), or a sugar-binding protein and a sugar (e.g., maltose).

The present invention includes uses of Fc regions, antibodies thereto, and inhibitory compounds of the present invention for the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

One embodiment is a therapeutic composition comprising at least one of the following therapeutic compounds: an inhibitory compound of the present invention, a mutein of the present invention, or an antibody of the present invention. Also included is a method to protect an animal from allergy or other abnormal immune responses. Such a method includes the step of administering a therapeutic composition of the present invention to the animal. As used herein, the ability of a therapeutic composition of the present invention to protect an animal from allergy or other abnormal immune responses refers to the ability of that composition to, for example, treat, ameliorate or prevent allergy or other abnormal immune responses. General characteristics of therapeutic compositions and methods to produce and use such therapeutic compositions are disclosed, for example, in WO 98/27208, *ibid.*, see, for example, page 39-47; such compositions and methods are incorporated by reference herein in their entireties. It is to be noted that although the compositions and methods disclosed in WO 98/27208, *ibid.*, relate to feline FcεRIα proteins, they are also applicable to therapeutic compositions of the present invention. Therapeutic compositions of the present invention are advantageous because they can be derived from analysis of 3-D models of the present invention and have improved functions, such as efficacy and safety.

Another embodiment is a diagnostic reagent comprising a mutein of the present invention. As used herein, a diagnostic reagent is a composition that includes a mutein that is used to detect allergy or other abnormal immune responses in an animal. Also included in the present invention are methods, including *in vivo* methods and *in vitro* methods, to (a) detect allergy or other abnormal immune response, or susceptibility thereto, in an animal, comprising use of a diagnostic reagent comprising a mutein of the present invention and (b) to enhance the performance of an IgE or FcR binding assay, said method comprising incorporating into the assay a mutein of the present invention. General characteristics of diagnostic reagents and methods to produce and use such diagnostic reagents are disclosed, for example, in WO 98/27208, *ibid.*, see, for example, page 2-39; such reagents and methods are incorporated by reference herein in their entireties. It is to be noted that although the reagents and methods disclosed in WO 98/27208, *ibid.*, relate to feline FcεRIα proteins, they are also applicable to

diagnostic reagents, kits and detection methods of the present invention. Muteins of the present invention are advantageous in such applications because of their enhanced affinity for antibodies, altered specificity, enhanced solubility and/or enhanced stability, enabling for example use in otherwise adverse conditions and longer shelf-life.

The following examples are provided for the purposes of illustration and are not intended to limit the scope of the invention.

EXAMPLES

Example 1.

This Example describes the production and analysis of a crystal and model of the present invention. It is to be noted that numbering of Fc-Cε3/Cε4 residues follows the convention of Dorrington et al, ibid.

The binding of soluble IgE to its high affinity receptor, FcεRI, is a requisite step in the cascade of events associated with the allergic response and anti-parasitic immunity[1-3]. Crosslinking of receptor-bound IgE by antigens triggers intracellular signaling events leading to effector cell activation[4]. This example describes the solution of a 2.3 Å crystal structure of the human IgE-Fc domains, Cε3 and Cε4, which bind to FcεRI, the coordinates of which are disclosed in Table 1. The IgE-Fc crystal structure reveals a large (~15°) tertiary rearrangement of the Cε3 domains when compared to IgG-Fc structures and the IgE-Fc bound to FcεRI. The free IgE-Fc adopts a more compact arrangement that places the Cε3 domains into close proximity in a "closed" configuration, obstructing receptor-binding loops. This IgE-Fc conformational change is mediated by three flexible segments that lie within the Cε3 domain and not by the interdomain connecting loop. The "closed" structure of the IgE-Fc highlights the potential for novel conformational variation in the effector domains of different antibody classes and suggests new strategies for the design of therapeutic compounds for the treatment of allergy and asthma.

The interaction of antibody Fc domains with cellular antibody receptors couples the diversity of the antibody repertoire to many effector cells of the immune system. Fc receptors specific for antibody subclasses, including IgE, IgG and IgA antibodies, are found on overlapping but distinct subsets of cells of the hematopoetic system and can thereby trigger distinct mechanisms of the immune response[1,4,5]. IgE-mediated immune reactions are implicated in parasitic infections, allergy and asthma.

IgE antibodies consist of two Fabs and an Fc that is formed by a dimer of three constant domains (Cε2, Cε3, and Cε4). Compared to IgG molecules, IgE has an additional constant domain (Cε2) that replaces the IgG linker region, while the IgE Cε3 and Cε4 domains are homologous to the IgG Cγ2 and Cγ3 domains. Intact IgE and Fc fragments bind with high affinity (K_D ~10^{-9}-10^{-10}M) to the alpha chain of FcεRI and

mutagenesis studies[6-11] have demonstrated that Cε3 domain residues are involved in binding to the receptor, consistent with the crystallographic studies of the IgE-Fc:FcεRIα complex. The IgE-Cε2 domains are not thought to be important for receptor binding, since constructs of the IgE-Cε3/Cε4 domains retain high affinity binding to the receptor.

In order to obtain protein for crystallographic studies, the C-terminal IgE-Fc domains, Cε3/Cε4, were expressed in insect cells and purified as described in the methods section. Crystals were obtained that diffract weakly using laboratory X-ray sources but diffract to 2.3Å using high energy synchrotron X-ray sources. The IgE-Fc Cε3/Cε4 structure was solved by an automated molecular replacement search strategy using ~12,000 distinct conformational variants of core models for the two immunoglobulin domains, in which the domain orientations were varied by rotation about three axes centered near the connecting loop between the two domains. A course (3° angular) search yielded a single promising solution that was further refined by finer domain rotations. The structure was subjected to rounds of refinement and building into simulated annealing composite omit electron density maps, giving the final statistics shown in Table 6. The Rfree and Rfactor are , respectively, with good geometry to 2.3 Å resolution.

The overall structure for the IgE Cε3/Cε4 domains is shown in Fig. 1a and 2a. The two immunoglobulin domains belong to the C1 set of antibody constant domains and are individually similar to the structures for the receptor-bound IgE-Fc and IgG-Fc domains shown in Figs. 1b, 2b and 1c, 2c, respectively. No density for residues N-terminal to V336 (the Cε2/Cε3 linker) are observed in the IgE-Fc structure, despite the fact that an interchain disulfide occurs in this region and can be shown to form biochemically. The Cε2/Cε3 linker becomes ordered and visible in electron-density maps upon binding FcεRI (see, for example, 60/189,853). Similar to the IgG-Fc, the Cε3 domains of the heavy chain dimer do not form any inter-chain contacts, while the Cε4 domains form an extensive dimer interface, burying ~1860 $Å^2$ of surface area. Conserved carbohydrate found at N394 in IgE, fills the cavity between the Cε3 and Cε4 domains and makes limited contacts across the dimer interface. In contrast to IgG-Fc structures, IgE carbohydrate can be removed and binding to FcεRI is retained[8].

The IgE-Fc crystal structure reveals a novel and compact closed conformation for the Fc domains. The relative dispositions of the two Cε3 domains with respect to each other and to the Cε4 domains is substantially different from IgG-Fc or the receptor-bound IgE-Fc structures (Fig. 1). The Cε3/Cε4 angle is more acute than that found between IgG-Fc Cγ2/Cγ3 domains or for the receptor-bound IgE-Fc (Fig. 1). The free IgE-Fc is more compact, as shown by its shorter overall height (Fig. 1a, ~7Å), with overall dimensions of 58x63x40Å as compared to 65x64x36Å for IgG-Fc (Fig. 1c) and to the dimensions of the receptor-bound IgE-Fc (Fig. 1b) (see, for example, 60/189,853). The Cε3 domains in the IgE-Fc structure also approach each other more closely, as shown by the distances between loop residues indicated in Fig. 2a. The distances between the first residue in strand A of the Cε3 or Cγ2 Ig domains can be readily compared, minimizing differences in distance due to loop flexibility. In IgG (Fig. 2c), this distance is ~22Å (varies some between IgG structures), in the receptor-bound IgE-Fc (Fig. 2b) this distance is ~23Å, while in the closed IgE (Fig. 2a) this distance is ~13Å. Overall, the receptor-bound IgE and IgG-Fc structures more closely resemble each other than the unbound IgE-Fc structure.

Although conformational differences in IgG-Fc structures have been noted[12,13], these are not as large as observed for the receptor-bound and closed IgE-Fc structures. Fig. 3 shows a superposition of nine different IgG structures along with the closed IgE-Fc structure observed here. The IgE-Fc lies significantly beyond the observed range of motion in IgG-Fc structures. A superposition of the receptor-bound and closed forms of the IgE-Fc is shown in Fig. 3, demonstrating the large conformational change observed. The AB helix of Cε3 and the interdomain linker residues remain relatively fixed with respect to the Cε4 domain, as shown by a superposition of the open and closed IgE conformations (Fig. 3). The largest IgG-Fc conformational differences are found in comparisons of human and mouse IgG-Fc structures that are 65% identical in sequence[12], potentially accounting for some of the conformational differences. In contrast, the IgE-Fc structures compared here demonstrate large conformational flexibility for a molecule of identical sequence.

An analysis of the IgE-Fc conformational difference is shown in Fig. 4a, in which comparison of the closed and open forms was carried out with the program

DynDom[14]. Dyndom groups residues that move as semi-rigid domains for proteins in different conformational states and identifies an interdomain screw axis and hinge residues for the IgE domain motion. The axis of the IgE bending motion is indicated by the arrow in Fig. 4a, with an approximately 15° rotation and 0.6Å translation relating the open and closed forms. The bend between the two domains does not occur in the interdomain region (residues 436 - 440) but rather occurs within the Cε3 domain itself. The residues that constitute the hinge lie above the Cε3-AB helix and include amino acids 342-344 (after strand A), 354-356 (before strand B), and 434-436 (after strand G) and are highlighted with light purple in Fig. 4a.

The structural basis for the difference in apparent flexibility in the IgG- and IgE-Fc domains is not simply based on sequence differences in the linker amino acids between the two immunoglobulin domains, given the potential for hinge motion in the three peptide segments identified by DynDom. The interdomain linker region and the AB helix remain relatively fixed in the comparison of closed and open IgE-Fc structures (Figs. 1c and 4a). At the C-terminal end of the AB helix, small structural changes account for a single residue insertion in IgG-Cγ2 sequences compared to IgE-Cε3 and these are not part of the hinge regions in IgE (Fig. 4b). In both IgE and IgG, the A and B β-strands of Cε3 or Cγ2 separate and do not hydrogen bond on either side of the AB helix, and it is in this region that the IgE bending appears to concentrate (Figs. 4a and 4b). Comparison of the IgG-Fc and IgE-Fc structures shows a concerted shift in the position of the IgE-Fc AB helix outwards from the Cε3/Cε4 interface, which may account for the greater rotational freedom in the IgE-Fc structures (Fig. 4b). In the closed IgE-Fc structure, the hinge residues immediately after the AB helix (amino acids 354-356) sterically clash with the superimposed IgG-Fc AB helix (Fig. 4b). Thus the closed conformation observed here for the IgE-Fc may be inaccessible to the IgG-Fc, because of the position of the IgG-Fc AB helix. Additional residues may also contribute to the conformational differences in IgG and IgE, such as the change of P257/P258 in IgG for R342/P343 in IgE in the A strand and the presence of P354 at the beginning of the IgE-AB helix. Differences in the phi/psi angles accessible to the double proline sequence in IgG could additionally stabilize the open configuration of IgG-Fcs. In contrast to human IgE-Fc, the mouse and rat sequences contain this double proline motif. It will be interesting to test if mutation of R342 for proline stabilizes the

open conformation as measured by solution techniques and if this mutation has an effect on the binding affinity for IgE receptors.

The large conformational change observed in the closed IgE-Fc structure reorients loops at the top of the Cε3 domains that interact with FcεRI. Fig. 4c quantifies these conformational differences by comparing the distance between pairs of Cα carbon atoms in the free IgE-Fc and the receptor-bound IgE-Fc. Loops that are involved in binding FcεRI are highlighted above the graph and these regions are observed to move by 10-14 Å between the bound and free forms of the IgE-Fc. Since the rotation axis lies near the base of the Cε3 domain (Fig. 4a), a gradient of increasing Cα displacements can be seen in this plot that corresponds to amino acids in the Cε3 beta strands. The peaks in the plot correspond to loops at the top of the Cε3 domain that show the largest displacements (Fig. 4c). The AB-helix in the Cε3 domain appears to be linked structurally to the Cε4 domains by this analysis as well as the domain-movements shown in Fig. 3.

The movement of the IgE-Fc receptor-binding loops by 10-14 Å suggests that these loops would be poorly positioned in the "closed" form to interact with the receptor-binding surface. Figs. 5a and 5b show surface representations of the FcR-binding loops of the Cε3 domain for the bound and free forms. The rotation of the Cε3 domains about this internal hinge reorients the receptor-binding surfaces. In the open, receptor-binding form, the Cε3 loops are exposed and together with the N-terminal linker residues to the Cε2 domains, form a crown-like structure that interacts with the broad and convex surface of FcεRI. In contrast, in the closed Fc conformation, the receptor-binding loops are reoriented to point towards each other across the IgE-Fc diad axis, forming a narrower inter-domain gap that cannot accommodate the binding of the receptor. The relatively large space separating Cγ2 domains in IgG and in the Cε3 domains of "open" form of IgE, becomes more of a cleft in the closed IgE-Fc (Fig. 5a).

The IgE-Fc conformation in solution is likely to be dynamic and the full range of Cε3 conformational mobility remains to be established. However, biophysical studies of IgE conformation in solution have previously suggested more compact models for the IgE conformation as compared to IgG antibodies. Neutron scattering studies of a three domain construct of the IgE-Fc (Cε2/Cε3/Cε4) are consistent with a

more compact structure than that of IgG-Fc in solution[15]. In addition, N-terminal to C-terminal distances for intact IgE have also been measured by fluorescence energy transfer (~71Å) and suggest a bent conformation for the antibody in solution, with less hinge-mediated flexibility as compared to IgG[16,17]. These studies may also be consistent with the more compact IgE-Fc conformation observed in the crystal structure reported here.

The observed conformational flexibility in the IgE-Fc may be important for unique aspects of IgE biological function. IgE-Fc flexibility may allow for induced-fit interactions with the FcεRI, contributing to the high affinity binding or may also be important in interactions with the low affinity IgE receptor, FcεRII (Fig. 6). FcεRII is a trimeric C-type lectin that is thought to interact with the IgE-Fc through two of the three lectin domains[18]. IgG antibodies do not interact with a corresponding lectin-like receptor, consistent with a potential biological role for IgE-Fc conformational variation in this unique antibody-receptor interaction. Finally, the observation of the closed IgE-Fc conformation provides a template for the design of new inhibitors of the IgE-FcεRI interaction (Fig. 6). Stabilization of the closed IgE-Fc conformation by the binding of small molecules, either at directly competitive or indirect allosteric sites, could block receptor association (Fig. 6), leading to a new class of therapeutic inhibitors for the treatment of IgE-mediated allergic diseases. The recent observation that in vitro selected peptides bind to the hinge region of the IgG-Fc, suggests the design of peptides that bind selectively to the closed IgE-Fc hinge to block FcεRI binding[19].

Methods

Expression and crystallization of the human IgE-Fc

The IgE-Fc Cε3/Cε4 was expressed in insect cells using the Pharmingen baculogold expression system. Briefly, DNA encoding the Cε3/Cε4 domains were subcloned into the pACgp67 expression vector and recombinant virus generated by established methods. IgE-Fc Cε3/Cε4 protein expression was monitored by a receptor-based ELISA assay and protein was purified by conventional techniques (ion exchange, gel filtration and hydroxyapatite chromatography) from 10-20 liters of supernatants of infected *T. ni* cells. The Fc construct codes for an N-terminal sequence (ADPCDSN) that includes four amino acids (ADPC) upstream of the native sequence beginning with

residue D330. The cysteine is displaced by one residue from the natural IgE-Fc cys328, but forms intramolecular disulfide binds in >95% of the isolated IgE-Fc.

Purified IgE-Fc was concentrated to 10 mg/ml in 10 mM Tris, pH 8.0, using an e280nm of 1.32 cm-1 (mg/mL)-1. Crystals were obtained using the hanging drop method by mixing 0.5 ml protein +0.5 ml of precipitant (25mM Sodium Acetate, pH 4.6, 33% (w/v) polyethylene glycol 4000). Crystals grew at room temperature in 1-3 days and were sensitive to small changes in salt or PEG concentration as well as temperature. Crystals were harvested into 25 mM Sodium Acetate, pH 4.6, 37% PEG 4000 and transferred to a cryoprotectant solution (harvest buffer plus 15% (v/v) ethylene glycol) for ~30 seconds prior to flash-freezing in liquid nitrogen. Crystals belong to the space group $P42_12$ with cell dimensions of a=b=105.6Å, c=47.1Å and $\alpha=\beta=\gamma=90^\circ$ and contain one Cε3/Cε4 chain per asymmetric unit of the crystal.

Crystal structure determination and refinement

Data from the IgE-Fc crystals was initially variably anisotropic, but improved substantially when crystals were treated with heavy atoms used for derivative screening, including platinum, mercury and other metals. Based on these onservations, crystals were treated with 1 mM copper (II) chloride prior to freezing and data collection. Although initial diffraction from native crystals was limited to ~3.0Å resolution and often exhibited split lattices, copper-treated crystals diffracted to at least 2.3Å resolution, with little anisotropy lattice problems. This improvement may be due to the oxidation of residual free cysteines (<5%) in the IgE-Fc N-terminal residues prior to freezing. Data were collected from these crsytals at SSRL beamline 7-1 using a Mar300 imaging plate system and at the Advanced Photon Source DND-CAT 5Idbeamline, using a MarCCD detector. Native and derivative data were processed and integrated using the HKL suite of programs.

Initial attempts at solving the crystal structure by Molecular Replacement (MR) methods failed, using a variety of models of IgE based on IgG-Fc structures, including individual Ig domains and superpositions of IgG Fc structures among others. MR searches were carried out with Amore, CNS/XPLOR and EPMR without success. Heavy atom searches were carried out with a wide range of compounds (27), concentrations (0.1-20mM) and pH ranges (4.6-8.5) but did not yield a well-behaved isomorphous derivative.

Since it was possible that the MR searches failed because of an altered conformation for the IgE-Fc as compared to the search model, a systematic exploration of the bend, twist and Cε3 rotation angles relative to Cε4 was undertaken. For this search, the Cγ2 and Cγ3 domains from the crystal structure of an intact mouse monoclonal antibody (PDB code 1IGT)[20] were used that were truncated to exclude non-homologous loops and side-chains, providing a model with 144 residues for 222 in the IgE-Fc construct. The two domains were translated to place the Cγ2/Cγ3 linker residues at the origin, with Cγ2 and Cγ3 oriented to allow a bending rotation to occur about the z-axis. Three rotations around X, Y and Z were applied to the Cγ2 domain, while leaving the Cγ3 fixed, using the program lsqkab from the CCP4 suite[21]. Approximately 12000 models were generated automatically and used in complete Molecular Replacement searches with the program Amore[21], taking ~10 days on 5 Silicon Graphics computers. The models covered an angular range of –30 to +40 degrees around the starting model with 3° increments in each rotation. A promising initial search solution was refined by restricting the search range and reducing the rotational stepsize to 0.5 degree increments. This fine search produced a model with a correlation coefficient of 38% and an Rfactor of 489% with data from 15-4 Å resolution. This model was subjected to rigid body refinement and a simulated annealing composite omit map was calculated to 3Å resolution using the program CNS[22]. Interpretable density was observed in regions omitted from the search model and errors in the model could be easily identified. Model building and refinement were continued using the programs O[23] and CNS[22]. The current refinement statistics for all data from 0-2.3Å resolution are collected in Table 6.

Table 6: Data Collection and Refinement

Data collection:

crystal (pH of harvest buffer)	wtcu3 (pH 6.5) wtcu1 (pH 7.5)	
Source	APS, DND-CAT (line=?)	SSRL, 7-1
Wavelength, energy	0.906 Å, 13.67 keV	1.08 Å, 11.48 keV
Resolution	2.30 Å (2.38 - 2.30 Å)†	2.60 Å (2.69 - 2.60 Å)†
Completeness	99.8% (99.5%)†	99.9% (99.0%)†
Total number of reflections	106,855	83,604
Unique reflections	12,340	8,586
Mosaicity	0.48°	0.65°
R_{merge}	5.4% (25.7%)†	6.6% (24.5%)†
Average redundancy	8.66 (> 7.1)†	9.74 (>7.4)†
<I/σI>	33.9 (10.6)†	13.9 (8.6)†

† last shell

References

1. Kinet, *Annu Rev Immunol* **17**, 931-972 (1999).
2. Metzger, *Immunol Rev* **125**, 37-48 (1992).
3. Sutton et al., *Nature* **366**, 421-428 (1993).
4. Daeron, *Annu Rev Immunol* **15**, 203-234 (1997).
5. Ravetch et al., *Annu Rev Immunol* **16**, 421-432 (1998).
6. Weetall et al., *Immunol* **145**, 3849-3854 (1990).
7. Nissim et al., *Embo J* **10**, 101-107 (1991).
8. Basu et al., *J Biol Chem* **268**, 13118-13127 (1993).
9. Henry et al., *Biochemistry* **36**, 15568-15578 (1997).
10. Presta et al., *J Biol Chem* **269**, 26368-26373 (1994).
11. Sayers et al., *Biochemistry* **37**, 16152-16164 (1998).
12. Harris et al., *J Mol Biol* **275**, 861-872 (1998).
13. Harris et al., *Adv Immunol* **72**, 191-208 (1999).
14. Hayward et al., *Proteins* **30**, 144-154 (1998).
15. Beavil et al., *Biochemistry* **34**, 14449-14461 (1995).
16. Zheng et al., *Biochemistry* **30**, 9125-9132 (1991).
17. Zheng et al., *Biochemistry* **31**, 7446-7456 (1992).
18. Shi et al., *Biochemistry* **36**, 2112-2122 (1997).
19. DeLano et al., *Science* **287**, 1279-1283 (2000).
20. Harris et al., *Nature* **360**, 369-372 (1992).
21. Collaborative Computational Project, *Acta Cryst.* **D50**, 760-763 (1994).
22. Brunger et al., *Acta Crystallogr D Biol Crystallogr* **54**, 905-921 (1998).
23. Jones et al., *Acta Crystallogr A* **47**, 110-119 (1991).

Example 2.

This Example describes the further refinement of the model described in Example 1. It is to be noted that numbering of Fc-Cε3/Cε4 (also referred to herein as Fc Cε3-Cε4) residues follows the convention of Dorrington et al, *ibid.*

IgE antibodies mediate anti-parasitic immune responses and the inflammatory reactions of allergy and asthma. This Example describes the solution of a crystal structure of the human IgE-Fc Cε3-Cε4 domains to 2.3 Å resolution, the coordinates of which are disclosed in Table 2 and Table 3. The IgE-Fc crystal structure reveals a novel, closed conformation for Fc domains. For example, the structure reveals a large rearrangement of the N-terminal Cε3 domains when compared to related IgG-Fc structures and to the IgE-Fc bound to its high affinity receptor, FcεRI. The IgE-Fc adopts a more compact, closed configuration that places the two Cε3 domains in close proximity, decreases the size of the interdomain cavity and obscures part of the FcεRI-binding site. Unique structural features of the Cε3-Cε4 interdomain interfaces are identified that may enable this conformational flexibility. Fc domain flexibility may allow IgE to form optimal interactions with both of its receptors, FcεRI and FcεRII. The structure of the IgE-Fc suggests new strategies for anti-allergy treatments including the design of molecules that act allosterically to block receptor binding.

A. Background

The functional diversity of the antibody repertoire involves both the creation of antigen-specific binding sites and the coupling of these specific binding sites to different effector mechanisms of the immune system. Within the antibody, these two functional roles are found on separable parts of the protein, the Fab and Fc regions. Two antigen-binding sites are contained within the Fab regions of antibodies, which are covalently linked through the antibody heavy chain to Fc effector domains (Harris et al., 1999; Padlan, 1994). The Fc domains provide specificity for the activation of downstream effector functions and are derived solely from constant domains of the antibody heavy chain. Isotype switching during B cell development produces immunoglobulins with identical antigenic specificity connected to different heavy chain constant regions that fall into five major classes or isotypes: IgA, IgD, IgE, IgG and IgM. Different Fc

isotypes interact with distinct sets of cellular receptors or soluble proteins to initiate specific defense mechanisms. Effector mechanisms are adapted for specific pathogens, for the physical location of an infection and for different stages of the immune response. Fc-associated effector mechanisms include phagocytosis, the initiation of cellular cytotoxicity and inflammation pathways, the activation of complement and the feedback regulation of antibody production (Daeron, 1997; Kinet, 1999; Ravetch and Clynes, 1998).

IgE antibodies interact through their Fc domains with two cellular receptors of the immune system, FcεRI and FcεRII (CD23). IgE antibodies bind to the high affinity receptor, FcεRI, on the surface of mast cells, basophils and eosinophils (Kinet, 1999; Metzger, 1992). Binding of polyvalent antigen by the receptor-bound IgE causes receptor aggregation, triggering cellular activation. On mast cells this leads to the release of histamine, inflammatory mediators and vasodilators. Mast cell reactions to environmental allergens are associated with the pathologies of allergy, asthma and anaphylaxis (Turner and Kinet, 1999). Activation of eosinophils by FcεRI provides defense mechanisms against parasitic infection (Gounni et al., 1994; Kinet, 1999), while FcεRI on dendritic cells can deliver IgE-bound antigen into the MHC class II antigen-presentation pathway (Maurer et al., 1998). IgE antibodies also interact with a lower affinity receptor, FcεRII, involved in antigen presentation, cellular cytotoxicity and the regulation of IgE production (Sutton and Gould, 1993). While FcεRI is homologous to a family of antibody receptors specific for IgE, IgG and IgA antibodies, FcεRII belongs to a different structural class of proteins and is uniquely associated with the IgE system.

IgE is the target of recent therapeutic approaches for asthma using humanized anti-IgE monoclonal antibodies (Chang, 2000; Jardieu and Fick, 1999). Antibodies directed against the IgE-Fc block receptor binding, leading to a decrease in receptor activation and expression levels and triggering a decrease in IgE serum levels. Structural studies of the IgE-Fc may provide new routes to improving anti-IgE therapies and to designing inhibitors for the treatment of a wide variety of atopic diseases.

IgE contains two antibody light chains associated with two heavy chains of the ε isotype. The three C-terminal constant domains of the heavy chain (Cε2, Cε3 and Cε4)

dimerize to form the Fc effector domains. Compared to IgG, IgE antibodies have an additional constant domain, Cε2 (Fig. 7a). The Cε3 and Cε4 domains are homologous to the IgG-Fc Cγ2 and Cγ3 domains, respectively, with 32% sequence identity between human IgE and IgG1 (Fig. 7b). Both intact IgE and IgE-Fc fragments (Cε2-Cε4, Cε3-Cε4) bind with high affinity (K_D ~10^{-9}-10^{-10}M) to FcεRI and mutagenesis studies have implicated Cε3-domain residues in mediating this interaction (Basu et al., 1993; Henry et al., 1997; Nissim et al., 1991; Presta et al., 1994; Weetall et al., 1990), as well as the binding to FcεRII (Shi et al., 1997; Sutton and Gould, 1993). IgE-Fc Cε3-Cε4 retains binding to both FcεRI (Basu et al., 1993; Henry et al., 1997; Young et al., 1995) and FcεRII (Shi et al., 1997), suggesting a minimal construct for structural studies.

Crystallographic studies of antibody Fc domains have previously been limited to the IgG class, leaving open many questions regarding the role of sequence and structural diversity in Fc-effector functions.

B. Structure Determination

The C-terminal domains of human IgE-Fc, Cε3-Cε4 (Fig. 7), were expressed in insect cells as described in Methods. The IgE-Fc Cε3-Cε4 protein contains three potential N-linked carbohydrate attachment sites, but only two are glycosylated in vivo, N371 and N394 (Basu et al., 1993; Young et al., 1995). Characterization of the Fc carbohydrate by endoglycosidase digestion, mass spectroscopy of tryptic peptides, and mutational analysis shows that high-mannose carbohydrate is attached to N394, which is a conserved glycosylation site in Fc domains. Although both deglycosylated IgE-Fc (Basu et al., 1993) and high-mannose IgE (Granato and Neeser, 1987) retain high binding affinity for FcεRI, deglycosylated IgE-Fc has a tendency to aggregate, making it a poor candidate for crystallographic studies (Basu et al., 1993).

The IgE-Fc was purified to homogeneity and crystallized. Crystals belong to space group $P42_12$ with cell dimensions a=b=105.6 Å, c=47.1 Å. The crystals contain a single IgE-Fc chain (half of the dimeric molecule) in the asymmetric unit, with the molecular dimer axis lying along a crystallographic dyad. The crystals diffract X-rays to 2.0 Å using synchrotron X-ray sources. Molecular replacement searches using a variety of IgG-Fc models were unsuccessful, as were heavy atom searches. The IgE-Fc Cε3-

Cε4 structure was solved by an automated molecular replacement search using ~12,000 distinct conformational variants of core models for the two Ig domains, systematically varying the angles relating the Cε3 and Cε4 domain models. Data collection and refinement statistics are shown in Table 7. The current R_{free} and R_{work} are 27.0% and 24.2%, respectively, to 2.3 Å resolution. There is no density for the ten amino-terminal residues of the protein (including the interchain disulfide) and the four C-terminal residues. In addition, the density for the Cε4 AB loop is poor.

Table 7: Data Collection and Refinement

Data Collection Statistics

Data Set	wtcu3 (pH 6.5)	wtcu1 (pH 7.5)
Source	APS DND 5-ID	SSRL 7-1
Wavelength (Å)	0.906	1.08
Resolution (Å)	30.0-2.30 (2.38 - 2.30)†	30.0-2.60 (2.69 - 2.60)†
Completeness	99.8% (99.5%)†	99.9% (99.0%)†
Unique reflections (Total)	12,340 (106,855)	8,586 (83,604)
Average redundancy	8.7 (>7.1)†	9.7 (>7.4)†
$\langle I/\sigma_I \rangle$	33.9 (10.6)†	13.9 (8.6)†
R_{merge}	5.4% (25.7%)†	6.6% (24.5%)†

Refinement (wtcu3):

Reflections, work (free): 11053 (1269)

R_{work}/R_{free}	Atoms (Total)	Protein Atoms	Water Molecules
24.2 / 27.0	1,763	1,618	145

Average B factor		RMS Deviations from Ideality	
Protein	Water	Bond angles	Bond lengths
51.8 Å^2	59.0 Å^2	1.77°	0.007 Å

Ramachandran (ϕ,ψ)

Favored	Allowed	Generous	Disallowed
87.3 %	12.2 %	0.0 %	0.6 %

† Values for the highest resolution shell are shown in parentheses

$R_{merge}=\Sigma|I_i-\langle I\rangle|/\Sigma|I|$, where I_i is the intensity of an individual reflection and $\langle I\rangle$ is the average intensity of that reflection.

$R_{work/free}= \Sigma||F_p|-|F_c||/\Sigma|F_p|$, where F_c is the calculated and F_p is the observed structure factor amplitude. R_{work} and R_{free} were calculated using the working set and test set reflections, respectively.

C. Description of the IgE Structure

The Cε3 and Cε4 domains of IgE belong to the C1 set of Ig constant domains (Murzin et al., 1995). While the IgE Cε3 and Cε4 domains are individually similar to IgG Cγ2 and Cγ3 domains, respectively, a structure-based sequence alignment of the IgE-Fc and IgG-Fcs reveals several changes in secondary structure (Fig. 7b). Compared to IgE, the IgG contains a single residue insertion (I253 in IgG1) that forms a bulge just after the Cγ2 AB helix. The IgE Cε3 domain lacks a C′ strand and the Cε4 domain has a poorly ordered AB loop in place of the AB helix in Cγ3. Two prolines (P381 and P454) may contribute to the disruption of these secondary structures by altering hydrogen bond capabilities.

A ribbon diagram of the IgE-Fc is shown in Fig. 8. As in IgG-Fcs, the upper domains (Cε3) of the IgE-Fc do not form any direct protein:protein contacts. The conserved carbohydrate attachment site (N394) faces the cavity between the Cε3 domains. While the observed electron density is consistent with glycosylation at this site, the poor quality of the density precludes modeling of carbohydrate. Inclusion of carbohydrate residues in the model did not decrease the R_{free} or improve the electron density maps. However, the electron density suggests that carbohydrate residues contact each other near the Fc dimer axis, forming the bottom of a narrow cleft between the Cε3 domains. The Cε4 domains form extensive contacts across the dimer interface, burying ~1,860 Å^2. Fourteen atomic contacts (< 4Å) formed between the Cε3 and Cε4 domains of a single chain bury 872 Å^2, and so bury a total of 1,744 Å^2 in the dimer.

No electron density for residues N-terminal to V336 (the Cε2-Cε3 linker region) is observed, despite the formation of the interchain disulfide in this region. These Cε2-Cε3 linker residues are ordered in the complex with FcεRI (Garman et al., 2000) and several of these residues interact with the receptor. While the absence of the Cε2 domains may contribute to the disorder of the Cε2-Cε3 linker in the free Fc, the asymmetric binding of linker residues to FcεRI suggests that flexibility is functionally important.

D. The IgE-Fc Adopts a Novel Conformation

The crystal structure of the IgE-Fc Cε3-Cε4 domains reveals a novel, closed conformation for antibody effector domains (Fig. 8). In the free IgE-Fc, the Cε3-Cε4 interdomain angle is more acute than that observed between homologous IgG-Fc domains (Deisenhofer et al., 1976; Harris et al., 1999) or in the FcεRI-bound IgE-Fc (open conformation, Garman et al., 2000). Both the relative dispositions of the two Cε3 domains with respect to each other and to the Cε4 domains is altered. In the closed structure, the IgE-Fc Cε3 domains are closer together and slightly rotated with respect to each other. A top view of the Cε3 and Cγ2 domains illustrates differences in the interdomain gap (Fig. 8b). In the IgE-Fc, the distance between the first residue of the Cε3 A strands is only 13 Å. The distance increases to 23 Å in the receptor-bound IgE-Fc, which is similar to the 22 Å observed between the Cγ2 domains in IgG2a-Fc (Harris et al., 1997). The Cε3 domains not only approach each other more closely, but they also lie closer to the Cε4 domains. For example, the top of the Cε3 domain (residue T396 in DE loop) is 23 Å from the top of the Cε4 domain (residue S491). The distance between the corresponding residues in IgG2a is 33 Å, and in the receptor-bound IgE-Fc (open form), the distance is 31 Å. Thus, in the change between the open and closed forms, the top of each Cε3 domain moves 10 Å towards the other Cε3 domain across the dimer axis and 8 Å towards the Cε4 domain of the same chain. The closer approach of the upper domains of IgE (Cε3) to the lower domains (Cε4) decreases the overall height of the IgE-Fc by ~7 Å compared to the IgG-Fc. The IgE-Fc conformational change is much greater than any differences observed among IgG-Fc crystal structures. Six crystal structures of the IgG-Fc provide nine different observations of a single chain of the IgG-Fc (in three structures, the two chains are constrained by crystallographic symmetry to be identical). These nine IgG-Fc chains, aligned via their Cγ3 domains, reveal IgG-Fc conformational variability as a family of Cγ2 positions (Fig. 9a). In the closed structure, the IgE Cε3 domain lies far outside the range of observed IgG-Fc conformations. When bound to FcεRI, the angle between the Cε3 and Cε4 domains increases and the Cε3 domains approach the observed positions for IgG Cγ2 domains. Some of the structural variation in the IgG-Fcs may be attributable to sequence differences. While the human

IgG structures share ~ 95% sequence identity and the mouse structures have ~67% identity, the largest difference in IgG Cγ2 positions occurs between the human and mouse structures which share ~ 64% identity (Harris et al., 1999). However, the largest conformational change occurs between the open and closed forms of the IgE-Fc, which are identical in sequence, demonstrating the inherent flexibility of the IgE-Fc.

E. Analysis of IgE- and IgG-Fc Conformational Flexibility

The IgE-Fc conformational change can be described by an axis relating the two Ig domains in the open and closed conformations. The program DynDom (Hayward and Berendsen, 1998) defines a rotation of ~13° and a translation of 1 Å about this axis (arrow in Fig. 9b). Surprisingly, the axis does not lie in the Cε3-Cε4 linker region (436-440) but rather within the Cε3 domain itself, near the Cε3-Cε4 domain interface. Hinge residues that mediate the conformational change lie at both ends of the Cε3 AB helix (residues 343-345 and 351-352) and adjacent to the Cε3-Cε4 linker (residues 435-436). None of the observed IgG-Fc structures exhibit such a large degree of flexibility. Three IgG-Fc structures have been solved in which the two Cγ2 domains of the same Fc exhibit different orientations with respect to their Cγ3 domains (1FC1 (Deisenhofer, 1981), 1IGY (Harris et al., 1998), and 1IGT (Harris et al., 1997)). Since the structural variation occurs within the same Fc, differences due to sequence variation are eliminated. For each structure, DynDom analysis identifies an axis near the Cγ2-Cγ3 interface that describes a motion of 6-7° between the two conformers (Fig. 9c). The orientations of the axes are different from each other and from that of the IgE-Fc, and they describe distinct movements (e.g. side-to-side) of Cγ2. However, none of the IgG motions match the open-to-closed conformational change seen in the IgE-Fc. The different location of the hinge axes and the much smaller range of motion displayed by the IgG-Fc suggest that the flexibility of Ig domains involves multiple factors.

The change in Cα coordinates between the closed and open conformations of the IgE-Fc is plotted in Fig. 9d. The changes are slightly different for the two Fc chains that bind asymmetrically to the FcεRI (Garman et al., 2000). The Cε3 AB helix (344-352) and the interdomain linker (436-440) remain relatively fixed with respect to the Cε4 domain, while the Cε3 EF helix residues (406-413) show Cα movements of up to

4 Å (Fig. 9a). Positional changes become greater further from the hinge, with the greatest displacement of Cε3 residues observed at the top of the Fc in the BC (363-368), DE (393-395) and FG (422-428) loops that bind to FcεRI (Fig. 9b). Residues in these loops move 7-16 Å between the open and closed conformations (Fig. 9c). Large differences are also observed in the A-strand adjacent to the Cε2-Cε3 linker.

F. IgE-Fc Carbohydrate

In both IgE and IgG, a conserved carbohydrate attachment site faces the cavity between the upper domains (Cε3 and Cγ2 respectively). Carbohydrate residues have not been included in the structure, but partial electron density for ~5 carbohydrate moieties can be observed at the conserved N394 site, branching after the core (-$GlcNAc_2Man$) into two arms. As in IgG, electron density for carbohydrate lies along the inner face of the protein, shielding hydrophobic residues from solvent (IgE residues Y339, L359, V361). The carbohydrate is not sequestered from solvent, however. In IgE, the carbohydrate attached to N394 can be removed by endoglycosidases under native conditions, suggesting that this region is at least transiently accessible in solution (Basu et al., 1993).

Carbohydrate is not required for high affinity binding to FcεRI, suggesting that it does not affect the conformation of the IgE-Fc significantly. IgA glycosylation is similarly not required for Fc-receptor binding (Mattu et al., 1998). In contrast, the presence of carbohydrate at a conserved N-linked attachment site in IgG (N297 in IgG1) is critical for maintaining Fc receptor-binding activities (Jefferis et al., 1998). Core glycosylation (-$GlcNAc_2Man_3$) of IgG, produced in mammalian, yeast and insect cells, is likely sufficient for this carbohydrate function (Jefferis et al., 1998). Functional and biophysical studies of IgG indicate that the carbohydrate moiety has only a limited and local effect on the Fc structure (Jefferis et al., 1998). A comparison of glycosylated and aglycosylated IgG-Fc with a panel of monoclonal antibodies showed no detectable epitope differences, suggesting that global structural changes were not occurring (Walker et al., 1989). ^{1}H-NMR has been used to study the influence of glycosylation on the structure of IgG-Fc. Histidine resonances were monitored in glycosylated and non-glycosylated IgG-Fc (Lund et al., 1990; Matsuda et al., 1990). Of the five histidines

monitored, only one near the conserved glycosylation site (H268 in the Cγ2 BC loop), reported any change in local environment. Histidines at the Cγ2-Cγ3 domain interface did not detect any structural differences. Based on the IgE-Fc:FcεRI crystal structure, the Cγ2 BC loop and DE loop containing the conserved glycosylation site are predicted to participate directly in FcγR interactions (Garman et al., 2000). Local structural changes in these loops could affect receptor binding.

G. Structural Changes at the Interdomain Interface

The interdomain interfaces of both IgG-Fc (Cγ2-Cγ3) and IgE-Fc (Cε3-Cε4) are important for Fc function, and structural differences in the interface may influence Fc domain flexibility. Four proteins bind to this region in IgG: neonatal Fc receptor (Burmeister et al., 1994), rheumatoid factor (Corper et al., 1997), Protein A (Deisenhofer, 1981), and Protein G (Sauer-Eriksson et al., 1995). Direct binding of proteins to this region in IgE has not been demonstrated. The binding site for FcεRII has been broadly mapped to the outer surface of Cε3 (Shi et al., 1997; Sutton and Gould, 1993), while the FcεRI binding site is distal to this interface and encompasses the Cε3 BC, DE, and FG loops as well as the Cε2-Cε3 linker (Garman et al., 2000; Henry et al., 1997; Presta et al., 1994). However, despite the fact that residues at the Cε3-Cε4 domain interface do not form direct contacts to the FcεRI, mutations in this region can have a profound effect on FcεRI binding. For example, substitution of IgE Cε3 AB helix residues with IgG Cγ2 AB helix residues disrupts binding, as does a single amino acid mutation, F329A (Presta et al., 1994), suggesting that interactions at the Cε3-Cε4 domain interface are important in maintaining a functional Fc. The AB helix (in Cε3 or Cγ2) mediates the majority of atomic contacts (atoms within 4 Å) between the Fc domains in both IgE and IgG (Fig. 7a). The AB helix contacts adjacent residues and residues in the EF helix of the upper domain. The AB helix also contacts residues in the C, F and G strands and FG loop of the lower Ig domain (Cε4 or Cγ3). Despite the central role of the AB helix in mediating interdomain contacts, AB helix residues are not conserved between IgE and IgG. Only one residue of the helix (εD347, γD262) is invariant (Fig. 7b). In addition, most of the residues that contact the AB helix are not conserved between IgE and IgG. The pattern of contacts made by AB helix residues is

different in IgE and IgG. In IgE, most of the contacts made by the AB helix are to residues of the lower (Cε4) domain (15/21 in the open conformation, Fig. 10a). Only one contact is made to the EF helix in the closed form and two additional contacts are formed in the open conformation (dashed lines). In IgG, the majority of the AB helix contacts (12/21) are to other residues within the same Cγ2 domain, with nine contacts to the lower Cγ3 domain. The Cγ2 AB helix forms extensive contacts to the EF helix. Two residues in particular, V263 and H329, form a network of nine contacts within the Cγ2 domain. There are two striking structural features unique to the IgG interdomain interface (Fig. 9a, 10d). A single residue insertion after the IgG Cγ2 AB helix, isoleucine 266, forms a distinct bulge at the end of the helix. This isoleucine, together with adjacent residues, forms part of a shallow pocket on the surface of the IgG (Fig. 10d). The second difference in IgG is the presence of a conserved histidine (H329) on the EF helix facing the AB helix. This histidine is completely conserved in IgGs across species and subtypes but is not found in other Ig isotypes. Histidine 329 forms five atomic contacts to the pocket formed by I266 and neighboring residues (Fig. 10d). The contacts made by H329 are maintained in all IgG-Fc structures, including a highly distorted Fab-Fc hinge-deleted IgG in which the AB helix no longer contacts the lower Ig domain and has shifted away from the Cγ2-Cγ3 domain interface (Guddat et al., 1993). In non-glycosylated IgG-Fc, the ^{1}H resonances of IgG H329 do not change (Lund et al., 1990; Matsuda et al., 1990), suggesting the preservation of these interactions.

In contrast, the corresponding residue in IgE, T407, makes two contacts to the AB helix in the open form (Fig. 10a, 10c) and makes only one contact and moves away from the AB helix in the closed form (Fig. 9a, 10a-c). In rat and mouse IgE sequences T407 is replaced by alanine, suggesting that the conservation of these side chain interactions is not important.

The extensive contacts formed by the IgG AB helix to other Cγ2 domain residues and the close packing of EF helix residue H329 to the AB helix distinguish the IgG Cγ2-Cγ3 interface. In IgG, the AB helix is more closely associated with the upper (Cγ2) domain than the lower (Cγ3) domain. In contrast, the IgE interface is characterized by

extensive interactions of the Cε3 AB helix residues with the lower Cε4 domain residues (Fig. 10a), and contacts with the EF helix are limited. In both IgE Cε3 and IgG Cγ2, the A and B strands separate and do not form hydrogen bonds on either side of the AB helix, allowing for some flexibility in the positioning of the AB helix. However, the flexibility may be limited in IgG by the extensive interactions of the Cγ2 AB and EF helices. In IgE, the limited contacts made between the Cε3 AB and EF helices may allow the helices to move independently.

H. Effect of the Conformational Change on the FcεRI Binding Site

The large conformational change of the IgE-Fc structure reorients loops in the Cε3 domains that interact with the high affinity receptor, FcεRI. The large movement of the FcεRI-binding loops suggests that they would be poorly positioned in the closed IgE-Fc structure to interact with the receptor. Fig. 11 shows a molecular surface representation of the open and closed Fc structures, with the receptor-binding residues highlighted in magenta. In the open form, the receptor-binding loops are exposed and the binding residues display a large concave surface that is available to interact with FcεRI. In the closed form, these loops are partially obscured and point towards each other across the IgE-Fc dyad axis, leaving only a narrow gap between the two Cε3 domains that cannot accommodate the binding of the receptor. While the Cε3 BC, DE and FG loops are largely inaccessible in the closed conformation, the disordered Cε2-Cε3 linker residues N-terminal to V336 could form an initial interaction with the receptor even in the closed IgE-Fc structure. Binding of the receptor to linker residues might shift the conformation of the Fc towards the open form, exposing the binding loops.

I. Structural Basis for the IgE-Fc Conformational Flexibility

The IgE-Fc structure reveals an unprecedented conformation for antibody effector domains with implications for Fc-receptor binding and therapeutic intervention in human disease. The structure of the closed IgE-Fc suggests that the effector domains of antibody isotypes may have evolved structural characteristics that are associated with isotype-specific biological functions. Structural features that could influence the flexibility of the IgE-Fc include the location and packing of hinge residues and the

specific interactions at the Cε3-Cε4 domain interface, such as the position and contacts of the Cε3 AB helix. Other factors that could potentially effect a change in conformation have been considered, such as the specific crystal-packing environment, the presence of high-mannose instead of complex carbohydrate, or the lack of the Cε2 domains. The present invention also includes the solution of a second crystal form of the IgE-Fc containing two IgE-Fc molecules in the asymmetric unit, both in the closed form. These five IgE-Fc chains all adopt a similar conformation, indicating that the closed conformation is not dictated by specific crystal-packing forces.

It remains to be established whether different carbohydrate structures at the conserved attachment site could influence the extent of the observed IgE-Fc conformational change. Biochemical studies of IgG suggest a limited structural role for the conserved carbohydrate in maintaining the overall three-dimensional arrangement of Fc domains, as discussed above. While functional studies of the IgE-Fc (FcεRIα binding) argue against a significant role for the conserved carbohydrate, structural studies of different IgE-Fc glycoforms may resolve this issue.

Biochemical and biophysical studies indicate that the IgE-Fc Cε2 domains form a separate structural unit from the Cε3-Cε4 structure solved here. The Cε2-Cε3 linker is susceptible to proteolytic digestion (Perez-Montfort and Metzger, 1982) and adopts an asymmetric conformation upon binding FcεRI (Garman et al., 2000), suggesting that it is accessible and flexible. The presence or absence of the Cε2 domains in the IgE-Fc does not significantly alter the binding constants or thermodynamic parameters ($\Delta G°$, $\Delta H°$, $\Delta S°$, and $\Delta Cp°$) of FcεRI binding (Keown et al., 1998). Therefore, the mode of binding to the receptor is likely to be similar for intact IgE-Fc and IgE-Fc Cε3-Cε4. Together, these results suggest that the Cε2 domains have little influence on the structure or conformation of the Cε3 domains.

Structural characteristics of the IgE Cε3-Cε4 domain interface, as compared to the IgG Cγ2-Cγ3 domain interface, likely enable the conformational flexibility of the IgE-Fc. The AB helix of the first domain (Cε3 or Cγ2) mediates most of the interdomain contacts in the Fc structure and is not conserved in sequence across the five different antibody classes. Packing contacts of the AB helix with the two Fc Ig domains

may differ significantly across antibody isotypes, potentially influencing Fc conformation, flexibility and function. The range of conformational flexibility of the Fc domains of different antibody classes could be linked to the evolution of isotype-specific effector functions. The more limited flexibility of IgG structures may reflect similarities in the structural requirements for FcγR and complement (C1q) interactions.

Other experimental evidence has suggested that IgE adopts a bent configuration in solution and that conformational changes may occur upon binding to FcεRI. The design and interpretation of these experiments could not have anticipated the specific IgE-Fc conformational change of the present invention. Binding of IgE-Fc to FcεRI (Keown et al., 1998) is characterized by a relatively large change in heat capacity ($\Delta Cp°$=-815 cal/mol K), which could be in part be caused by IgE-Fc conformational changes. In contrast, binding of IgG-Fc to its homologous low affinity receptor, FcγRIII, exhibits a smaller change in heat capacity ($\Delta Cp°$=-360 cal/mol K). Fluorescence energy transfer experiments have shown that the average distance between the N- and C- termini of the IgE is only ~70 Å, a distance that is possible only if the IgE bends significantly out of the plane of the typical antibody Y- or T-shape (Zheng et al., 1991). Neutron scattering studies have shown that the intact IgE-Fc (Cε2-Cε4) has a significantly more compact shape than a linear arrangement of the domains would allow (Beavil et al., 1995), suggesting that a bend occurs within the IgE-Fc region. The IgE-Fc crystal structure supports the interpretation of bending of the intact IgE at the Cε2-Cε3 linker region, and may provide a better model for the analysis of the neutron scattering data. Experimental tests of IgE flexibility can now be developed based on the structure.

J. Biological and Therapeutic Implications for IgE-Fc Conformational Flexibility

Conformational flexibility in the IgE-Fc may be important for unique aspects of IgE biological function. IgE-Fc flexibility may allow induced-fit interactions with FcεRI, contributing to the high affinity binding, and may be important for interactions with the low affinity IgE receptor, FcεRII (Fig. 12). FcεRII is a trimeric C-type lectin that is thought to interact with the IgE-Fc through two of its three lectin domains (Shi et

al., 1997). IgG antibodies do not have a corresponding lectin-like receptor, suggesting that the conformational flexibility of the IgE-Fc may be important for this unique antibody-receptor interaction.

The existence of a closed conformation for the IgE-Fc and the demonstration that the open form binds to the high affinity receptor (Garman et al., 2000) suggest new strategies for the design of inhibitors of the IgE:FcεRI interaction (Fig. 12). Monoclonal antibodies that bind the IgE-Fc and block interactions with FcεRI have demonstrated the therapeutic potential of this approach for the treatment of allergy and asthma (Chang, 2000; Jardieu and Fick, 1999). Stabilization of the closed IgE-Fc conformation by the binding of molecules, either at directly competitive or indirect allosteric sites, could block receptor association, leading to a new class of therapeutic inhibitors for the treatment of IgE-mediated allergic diseases. The IgE Cε3-Cε4 domain interface may provide a target for the binding of small *in vitro*-selected ligands, as shown for the IgG-Fc (DeLano et al., 2000), that have the potential to act as allosteric inhibitors of receptor binding (Fig. 13). The closed conformation of the IgE-Fc provides the foundation for exploring new routes to alleviating atopic disease and exploring the functional role of Fc domain flexibility in biological effector mechanisms.

K. Methods

1. Expression and purification of the human IgE-Fc.

The expression, purification and characterization of the IgE-Fc from insect cells was performed as described in Example 1.

2. Crystallization and treatment of crystals

Purified IgE-Fc was concentrated to 10 mg/ml in 10 mM Tris, pH 8.0, using an ε_{280nm} of 1.32 cm^{-1} $(mg/ml)^{-1}$. Crystals were grown in hanging drops using the vapor diffusion method by mixing 0.5 µl protein and 0.5 µl of precipitant (25 mM sodium acetate, pH 4.6, 33% polyethylene glycol [PEG] 4000). Crystals grew at 22°C in 1-3 days and were sensitive to small changes in salt or PEG concentration and temperature. Crystals were harvested into 25 mM sodium acetate, pH 4.6, 37% PEG 4000, transferred briefly (< 30s) to cryoprotectant solution (harvest solution plus 15% (v/v) ethylene glycol) and cooled rapidly in liquid nitrogen. Crystals belong to the space group $P42_12$

(a=b= 105.6 Å, c=47.1 Å) and contain one Cε3-Cε4 chain per asymmetric unit. Crystals were transferred serially to higher pH harvest solutions to facilitate metal binding and redox chemistry. Heavy atom screening (~100 conditions) with a wide range of compounds (27), concentrations (0.1-20 mM) and pH ranges (4.6-8.5) did not yield an isomorphous or anomalous derivative. However, mercury- or platinum-treated crystals diffracted better than native crystals. Based on these observations, crystals were treated with 1 mM copper (II) chloride prior to cooling and data collection. Native crystals diffracted to ~2.8 Å resolution using a synchrotron source and displayed strong anisotropy and, occasionally, split lattices. Copper-treated crystals diffracted to at least 2.0 Å resolution, with little or no anisotropy. We and others (Basu et al., 1993) have observed that a small fraction of the IgE-Fc does not form the interchain disulfide. The copper II may have oxidized the remaining free cysteines to the disulfide.

3. Data collection, molecular replacement and refinement.

Data sets were collected at −160°C from copper-treated crystals at SSRL beamline 7-1 (wtcu1) using a Mar300 imaging plate system and at the Advanced Photon Source DND-CAT 5ID beamline (wtcu3) using a MarCCD detector. The data were processed and integrated using the HKL suite of programs (Otwinowski and Minor, 1997). Initial molecular replacement (MR) searches with AMoRe (Collaborative Computational Project, 1994), CNS/XPLOR (Brünger et al., 1998) and EPMR (Kissinger et al., 1999) failed, using a variety of models of IgE based on IgG-Fc structures, including individual Ig domains and a composite model incorporating seven IgG structures. A systematic exploration of the bend, twist and rotation angles of Cε3 relative to Cε4 was then undertaken. A model was constructed from the Cγ2-Cγ3 domains derived from an intact IgG structure (murine IgG2a, PDB entry 1IGT (Harris et al., 1997)), by truncating loops and non-homologous side-chains, resulting in a 144 residue model for the 222 residue IgE-Fc. The Cγ2-Cγ3 linker region of the model was placed at the origin, with Cγ2 and Cγ3 oriented to allow bending to occur about the Z-axis. Rotations around X, Y and Z were applied to the Cγ2 domain (3° steps), while leaving the Cγ3 fixed. Approximately 12,000 models were generated automatically with the program lsqkab (Collaborative Computational Project, 1994) and used in complete

AMoRe (Collaborative Computational Project, 1994) searches with the 15-4 Å data from crystal wtcu1 (Table 7). The models covered an angular range of -30 to +40 degrees around the starting IgG2a structure. A single solution, ~17° from the starting structure, was found and improved by a local search using 1.0° rotational increments. The finer search yielded a solution with a correlation coefficient of 38% and an R_{factor} of 48.9%. Cycles of model building into simulated-annealing composite-omit electron density maps and refinement were continued with the higher resolution data from crystal wtcu3 using the programs O (Jones et al., 1991) and CNS (Brünger et al., 1998). Refinement was performed against all data from 30-2.3 Å using |F|>0 and an anisotropic bulk solvent correction. Only refinement steps that decreased the R_{free} were accepted. The model includes residues 336-543 and lacks 10 N-terminal and 4 C-terminal residues present in the construct. The receptor binding loops (Cε3 BC, DE, and FG loops) have weaker density and higher B-factors than most of the other residues. Density for the Cε4 AB loop is particularly poor, and this loop was modeled sterically. All of the residues lie within the accepted regions of the Ramachandran plot, with the exception of N481. There is good density for this residue, however, which is in a tight turn that lacks a Gly, Ala, or Ser residue. While some density was for carbohydrate was observed at the N394 site, attempts to build carbohydrate did not improve the R_{free} or the electron density maps, and so it was not included in the model. There is no electron density for the carbohydrate attached to the N371 site. The current refinement statistics are summarized in Table 7. Figures were made using the programs MOLSCRIPT (Kraulis, 1991), GRASP (Nicholls et al., 1991) and Raster 3D (Merritt and Bacon, 1997).

L. References

Basu et al. (1993), *J. Biol. Chem. 268*, 13118-27.

Beavil et al. (1995), *Biochemistry 34*, 14449-61.

Brünger et al. (1998), *Acta Crystallogr. D. Biol. Crystallogr. 54*, 905-21.

Burmeister et al. (1994), *Nature 372*, 379-83.

Chang (2000), *Nat. Biotechnol. 18*, 157-162.

Collaborative Computational Project, No. 4 (1994), *Acta Cryst. D 50*, 760-763.

Corper et al. (1997), *Nat. Struct. Biol. 4*, 374-81.

Daeron (1997), *Annu. Rev. Immunol. 15*, 203-34.

Deisenhofer (1981), *Biochemistry 20*, 2361-70.

Deisenhofer et al. (1976), *Hoppe-Scyler's Z. Physiol. Chem. 357*, 1421-34.

DeLano et al. (2000), *Science 287*, 1279-83.

Dorrington et al. (1978), *Immunol. Rev. 41*, 3-25.

Garman et al. (2000), *Nature 406*, 259-266

Gounni et al. (1994), *Nature 367*, 183-6.

Granato et al. (1987), *Mol. Immunol. 24*, 849-55.

Guddat et al. (1993), *Proc. Natl. Acad. Sci. USA 90*, 4271-5.

Harris et al. (1997), *Biochemistry 36*, 1581-97.

Harris et al. (1997), *Adv. Immunol. 72*, 191-208.

Harris et al. (1999), *J. Mol. Biol. 275*, 861-72.

Hayward et al. (1998), *Proteins 30*, 144-54.

Henry et al. (1997), *Biochemistry 36*, 15568-78.

Jardieu et al. (1999), *Int. Arch. Allergy Immunol. 118*, 112-5.

Jefferis et al.(1998), *Immunol. Rev. 163*, 59-76.

Jones et al.(1991), *Acta Crystallogr. A 47*, 110-9.

Kelly et al.(1998), *J. Immunol. 161*, 6696-704.

Keown et al. (1998), *Biochemistry 37*, 8863-9.

Kinet, J. P. (1999), *Annu. Rev. Immunol. 17*, 931-72.

Kissinger et al.(1999), *Acta Crystallogr. D Biol. Crystallogr. 55*, 484-91.

Kraulis, P. J. (1991), *J. Appl. Cryst. 24*, 946-950.

Lund et al. (1990), *Mol. Immunol. 27*, 1145-53.

Matsuda et al. (1990), *Mol. Immunol. 27*, 571-9.

Mattu et al. (1998), *J. Biol. Chem. 273*, 2260-72.

Maurer et al. (1998), *J. Immunol. 161*, 2731-9.

Merritt et al. (1997), *Methods in Enzymology 277*, 505-24.

Metzger et al. (1992), *Immunol. Rev. 125*, 37-48.

Murzin et al. (1995), *J. Mol. Biol. 247*, 536-40.

Nicholls et al. (1991), *Proteins 11*, 281-96.

Nissim et al. (1991), *EMBO J. 10*, 101-7.

Otwinowski et al. (1997), In Methods in Enzymology: Macromolecular Crystallography, part A, C.W. Carter, Jr. & R.M. Sweet, Eds., Academic Press, pp. 307-326.

Padlan, E. A. (1994), *Mol. Immunol. 31*, 169-217.

Perez-Montfort et al. (1982), *Mol. Immunol. 19*, 1113-25.

Presta et al. (1994), *J. Biol. Chem. 269*, 26368-73.

Ravetch et al. (1998), *Immunol. 16*, 421-32.

Sauer-Eriksson et al. (1995), *Structure 3*, 265-78.

Shi et al. (1997), *Biochemistry 36*, 2112-22.

Sutton et al. (1993), *Nature 366*, 421-8.

Turner et al. (1999), *Nature 402*, B24-30.

Walker et al. (1989), *Biochem. J. 259*, 347-53.

Weetall et al. (1990), *J. Immunol. 145*, 3849-54.

Young et al. (1995), *Protein Eng. 8*, 193-9.

Zheng et al. (1991), *Biochemistry 30*, 9125-32.

While the various embodiments of the present invention have been described in detail, it is apparent that modifications and adaptations of those embodiments will occur to those skilled in the art. It is to be expressly understood, however, that such modifications are adaptations are within the scope of the present invention, as set forth in the following claims.

What is claimed is:

1. A three-dimensional model selected from the group consisting of: (a) a three-dimensional model of a human IgE Fc region comprising Cε3 and Cε4 domains (Fc-Cε3/Cε4), wherein said model substantially represents the atomic coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5; and (b) a three-dimensional model comprising a modification of said model of (a), wherein said modification represents an antibody Fc region that binds to a FcεRIα protein.

2. The model of Claim 1, wherein said model is represented by a method selected from the group consisting of listing the coordinates of all atoms comprising said model, providing a physical three-dimensional model, imaging said model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of said model.

3. The model of Claim 1, wherein said model identifies the solvent accessibility of amino acid residues of said protein listed in a Table selected from the group consisting of Table 2 and Table 6.

4. The model of Claim 1, wherein said model represents an antibody that binds to a FcεRIα protein with an affinity that is at least equivalent to the affinity of a human IgE antibody Fc-Cε3/Cε4 region for the extracellular domain of a FcεRIα protein selected from the group consisting of a human FcεRIα protein, a canine FcεRIα protein, a feline FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein and a rat FcεRIα protein.

5. The model of Claim 1, wherein said model represents a Fc-Cε3/Cε4 region of an antibody selected from the group consisting of a human IgE antibody, a canine IgE antibody, a feline IgE antibody, an equine IgE antibody, a murine IgE antibody, and a rat IgE antibody.

6. The model of Claim 1, wherein said model comprises a three-dimensional model of a Fc-Cε3/Cε4 region of an IgE antibody other than human IgE.

7. The model of Claim 6, wherein said model is produced by incorporating all or any part of the amino acid sequence of the Fc-Cε3/Cε4 region of said other IgE

antibody into a three-dimensional model of said human Fc-Cε3/Cε4 region to produce said model of Claim 6.

8. The model of Claim 1, wherein said model represents a FcεRIα binding domain.

9. The model of Claim 1, wherein said model is produced by a method comprising:

(a) crystallizing a Fc-Cε3/Cε4 region of a human IgE antibody;

(b) collecting X-ray diffraction data from said crystallized region; and

(c) determining said model from said data and amino acid sequence of said region.

10. The model of Claim 9, wherein said Fc-Cε3/Cε4 region has amino acid sequence SEQ ID NO:2.

11. The model of Claim 1, wherein said model has a three-dimensional structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 10 angstroms when superimposed on said three-dimensional model substantially represented by the atomic coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5.

12. The model of Claim 1, wherein said modification comprises an antibody Fc region that shares at least about 30% amino acid sequence homology with an IgE Fc region having amino acid sequence SEQ ID NO:2.

13. The model of Claim 1, wherein said model represents an IgE Fc region having an improved function selected from the group consisting of increased stability compared to the stability of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2, increased affinity for a FcεRIα protein compared to the FcεRIα affinity of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2, altered substrate affinity compared to the affinity for human FcεRIα of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2, and increased solubility compared to the solubility of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2.

14. The model of Claim 1, wherein said model is used to identify an inhibitor of the selective binding between a FcεRIα protein and an IgE antibody.

15. The model of Claim 1, wherein said model identifies crystal contacts between a FcεRIα protein and a Fc-Cε3/Cε4 region of an IgE antibody.

16. The model of Claim 1, wherein Cε3 and Cε4 domains of said antibody Fc region are oriented in a manner as specified by the structural coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5.

17. The model of Claim 1, wherein a structure selected from the group consisting of the interdomain groove between the two Cε3/Cε4 domains of said antibody Fc region, the hinge between Cε3 and Cε4 domains of said antibody Fc region, and a loop involved in FcεRIα binding is oriented in a manner as specified by the structural coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5.

18. The model of Claim 17, wherein said FcεRIα binding loop is selected from the group consisting of the linker between Cε2 and Cε3, BC loop of Cε3, DE loop of Cε3, and FG loop of Cε3.

19. The model of Claim 1, wherein the distance between the two Cε3 domains ranges from about 10 angstroms to about 25 angstroms.

20. The model of Claim 1, wherein the distance between the two Cε3 domains is about 13 angstroms.

21. A method to produce a three-dimensional model of a Fc-Cε3/Cε4 region of a human IgE antibody, said method comprising representing amino acids of said region at substantially the atomic coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5.

22. The method of Claim 21, wherein said model is represented by a method selected from the group consisting of listing the coordinates of all atoms comprising said model, providing a physical three-dimensional model, imaging said model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of said model.

23. A method to produce a three-dimensional model of a FcεRIα binding domain other than a human FcεRIα binding domain represented by the three-dimensional model substantially representing the atomic coordinates specified in a Table

selected from the group consisting of Table 1, Table 4 and Table 5, said method comprising homology modeling.

24. The method of Claim 23, wherein said method comprises incorporating at least a portion of the amino acid sequence of said other FcεRIα binding domain into said three-dimensional model substantially representing the atomic coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5 to produce said model of said other FcεRIα binding domain.

25. The method of Claim 23, wherein said method comprises orienting said immunoglobulin domains such that the distance between the two Cε3 domains ranges from about 10 angstroms to about 25 angstroms.

26. An isolated crystal of a Fc-Cε3/Cε4 region of a human IgE antibody.

27. The crystal of Claim 26, wherein said region has amino acid sequence SEQ ID NO:2.

28. The crystal of Claim 26, wherein said crystal belongs to space group spacegroup $P42_12$.

29. The crystal of Claim 26, wherein said crystal has cell dimensions of 105.6 angstroms x 105.6 angstroms x 47.1 angstroms, alpha=beta=gamma=90 degrees, and contains one Cε3/Cε4 chain per asymmetric unit of the crystal.

30. The crystal of Claim 26, wherein said Fc-Cε3/Cε4 region is produced in insect cells.

31. The crystal of Claim 26, wherein said crystal diffracts X-rays to a resolution of about 2.3 angstroms.

32. A method to produce an isolated crystal of a Fc-Cε3/Cε4 region of a human IgE antibody, said method comprising vapor diffusion..

33. The method of Claim 32, wherein said Fc-Cε3/Cε4 region has amino acid sequence SEQ ID NO:2.

34. The method of Claim 32, wherein said crystal belongs to a space group selected from the group consisting of spacegroup $P42_12$ having cell dimensions of 105.6 angstroms x 105.6 angstroms x 47.1 angstroms, alpha=beta=gamma=90 degrees.

35. The method of Claim 32, wherein said Fc-Cε3/Cε4 region is produced in insect cells.

36. The method of Claim 32, wherein said crystal diffracts X-rays to a resolution of about 2.3 angstroms.

37. An isolated Fc-Cε3/Cε4 protein selected from the group consisting of: (a) a protein consisting of SEQ ID NO:2; and (b) an isolated protein that is structurally homologous to a protein of (a), wherein said protein of (b) binds to a FcεRIα protein.

38. The protein of Claim 37, wherein said protein is produced in insect cells.

39. The protein of Claim 37, wherein said Fc-Cε3/Cε4 protein is selected from the group consisting of a human Fc-Cε3/Cε4 protein, a canine Fc-Cε3/Cε4 protein, a feline Fc-Cε3/Cε4 protein, an equine Fc-Cε3/Cε4 protein, a murine Fc-Cε3/Cε4 protein, and a rat Fc-Cε3/Cε4 protein.

40. A nucleic acid molecule comprising a nucleic acid sequence that encodes said protein of Claim 37.

41. A recombinant molecule comprising a nucleic acid sequence of Claim 40.

42. A recombinant virus comprising a nucleic acid sequence of Claim 40.

43. A recombinant cell comprising a nucleic acid sequence of Claim 40.

44. A method to produce a protein comprising culturing a recombinant cell of Claim 43.

45. A method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein, said method comprising using a three-dimensional model of a Fc-Cε3/Cε4 region of a human IgE to identify said compound, wherein said model substantially represents the atomic coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5.

46. The method of Claim 45, wherein said compound interacts with a region of said model selected from the group consisting of the FcεRIα binding domain, the interdomain groove between the two Cε3/Cε4 domains of said antibody Fc region, the hinge between Cε3 and Cε4 domains of said antibody Fc region, and a region of a Cε3 or Cε4 domain, the relative position of which changes by greater than 1 angstrom between closed and receptor-bound Fc-Cε3/Cε4 conformations.

47. The method of Claim 46, wherein the distance between the two Cε3 domains of said Fc-Cε3/Cε4 region ranges from about 10 to about 25 angstroms.

48. The method of Claim 46, wherein the distance between the two Cε3 domains of said Fc-Cε3/Cε4 region is about 13 angstroms.

49. The method of Claim 45, wherein said compound interacts with a region of said model selected from the group consisting of a linker between Cε2 and Cε3, a BC loop of Cε3, a DE loop of Cε3, and a FG loop of Cε3, a loop or strand defining the interdomain groove, a AB helix of Cε3 and, a region lying above said AB helix of Cε3.

50. The method of Claim 45, wherein said compound interacts with an amino acid selected from the group consisting of: (a) a residue having a position in SEQ ID NO:2 selected from the group consisting of position 4, 7, 8, 9, 10, 11, 17, 18, 19, 20, 21, 22, 23, 24, 29, 30, 31, 37, 38, 39, 68, 69, 70, 99, 100, 101, 102, 109, 110, and 111; and (b) a surface residue within about 10 angstroms of any of said residues of (a).

51. The method of Claim 45, wherein said compound interacts with an amino acid selected from the group consisting of: (a) a residue having a position in SEQ ID NO:2 selected from the group consisting of position 4, 7, 8, 9, 10, 11, 37, 38, 39, 68, 69, 70, 99, 100, 101, and 102; (b) a residue in a region of a Cε3 or Cε4 domain, the relative position of which changes by greater than 1 angstrom between closed and receptor-bound Fc-Cε3/Cε4 conformations; and (c) a surface residue within about 10 angstroms of any of said residues of (a) or (b).

52. The method of Claim 45, wherein said compound inhibits the ability of an IgE antibody to convert from a closed conformation to a receptor-bound conformation.

53. The method of Claim 52, wherein said closed conformation comprises a Fc-Cε3/Cε4 region wherein the distance between said Cε3 domains ranges from about 10 to about 25 angstroms.

54. The method of Claim 52, wherein said receptor-bound conformation comprises a Fc-Cε3/Cε4 region wherein the distance between said Cε3 domains ranges from about 20 to about 30 angstroms.

55. The method of Claim 45, wherein said method comprises:

(a) generating said model, or a model of a FcεRIα binding domain of said Fc-Cε3/Cε4 region, on a computer screen;

(b) generating the spacial structure of a compound to be tested; and

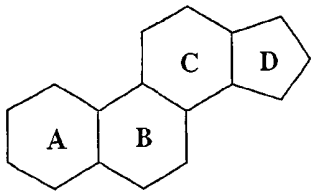
(c) testing to determine if said compound interacts with said FcεRIα binding domain, wherein such an interaction indicates that said compound is capable of inhibiting said binding of an IgE antibody to a FcεRIα protein.

56. The method of Claim 45, wherein said method further comprises using a three-dimensional model selected from the group consisting of a three-dimensional model of an extracellular domain of a human high affinity FcεRIα protein and a three-dimensional model of a complex between an extracellular domain of a human high affinity FcεRIα protein and a Fc-Cε3/Cε4 region of a human IgE antibody to identify said compound.

57. The method of Claim 45, wherein said inhibitory compound has a structure corresponding to at least a region of the space predicted by said model.

58. The method of Claim 45, wherein said inhibitory compound is a tetracyclic hydrocarbon perhydrocyclopentanophenanthrene.

59. The method of Claim 45, wherein said inhibitory compound comprises the following structural formula:



60. The method of Claim 45, wherein 3-[3-(cholamidopropyl) dimethylammonio]-1-propane-sulfonate (CHAPS) is used as a lead to identify said inhibitory compound.

61. The method of Claim 45, wherein said inhibitory compound is selected from the group consisting of a bivalent compound that interacts with the two Cε3/Cε4 domains with high affinity and a compound that is sufficiently large to bind the interdomain groove.

62. An inhibitory compound identified in accordance with the method of Claim 45.

63. A therapeutic composition comprising an inhibitory compound of Claim 62.

64. A method to protect an animal from allergy, said method comprising administering to said animal an inhibitory compound of Claim 62.

65. A mutein that binds to an IgE binding domain of a FcεRIα protein, wherein said mutein has an improved function compared to a Fc-Cε3/Cε4 protein comprising amino acid sequence SEQ ID NO:2, wherein said improved function is selected from the group consisting increased stability compared to the stability of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2, increased affinity for a FcεRIα protein compared to the FcεRIα affinity of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2, altered substrate affinity compared to the affinity for human FcεRIα of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2, and increased solubility compared to the solubility of a human IgE Fc region comprising amino acid sequence SEQ ID NO:2, wherein said mutein is produced by a method comprising:

(a) analyzing a three-dimensional model substantially representing the atomic coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5 to identify at least one amino acid of the Fc-Cε3/Cε4 protein represented by said model which if replaced by a specified amino acid would effect said improved function of said Fc-Cε3/Cε4 protein; and

(b) replacing said identified amino acid(s) to produce said mutein having said improved function.

66. A method to improve a function of an antibody comprising a Fc-Cε3/Cε4 region, said improved function being selected from the group consisting of increased stability, increased affinity for an IgE binding domain of a FcεRIα protein, altered substrate specificity, and increased solubility, said method comprising:

(a) analyzing a three-dimensional model substantially representing the atomic coordinates specified in a Table selected from the group consisting of Table 1, Table 4 and Table 5 to identify at least one amino acid of the Fc-Cε3/Cε4 region represented by said model which if replaced by a specified amino acid improves at least one of said functions of said Fc-Cε3/Cε4 region; and

(b) replacing said identified amino acid(s) to produce a mutein having at least one of said improved functions.

67. A composition selected from the group consisting of a FcεRIα binding domain, an interdomain groove between the two Cε3/Cε4 domains of said antibody Fc region, a hinge between Cε3 and Cε4 domains of said antibody Fc region, and a region of a Cε3 or Cε4 domain, the relative position of which changes by greater than 1 angstrom between closed and receptor-bound Fc-Cε3/Cε4 conformations.

68. The composition of Claim 67, wherein said composition is selected from the group consisting of a linker between Cε2 and Cε3, a BC loop of Cε3, a DE loop of Cε3, and a FG loop of Cε3, a loop or strand defining the interdomain groove, a AB helix of Cε3 and, a region lying above said AB helix of Cε3.

69. An isolated nucleic acid molecule encoding a protein of Claim 67.

IgE Fc Cε3-Cε4
Closed form

Fig. 1a

IgE Fc Cε3-Cε4
Open form

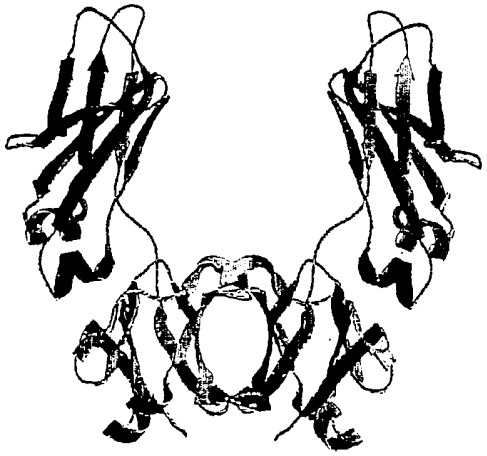


Fig. 1b

IgG Fc

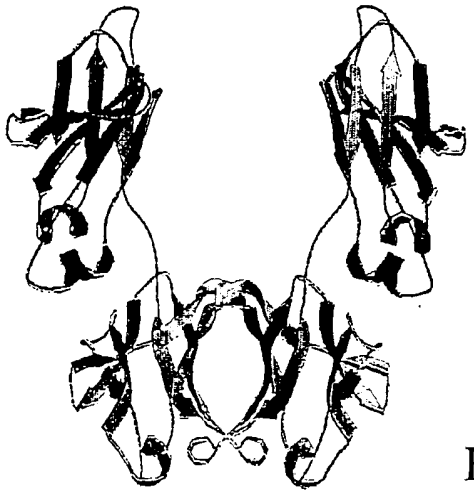


Fig. 1c

Closed IgE-Fc

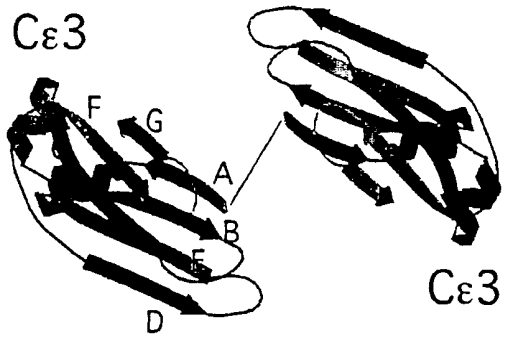


Fig. 2a

Open IgE-Fc

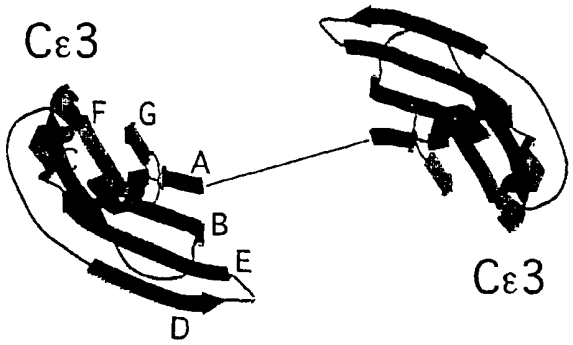


Fig. 2b

IgG-Fc

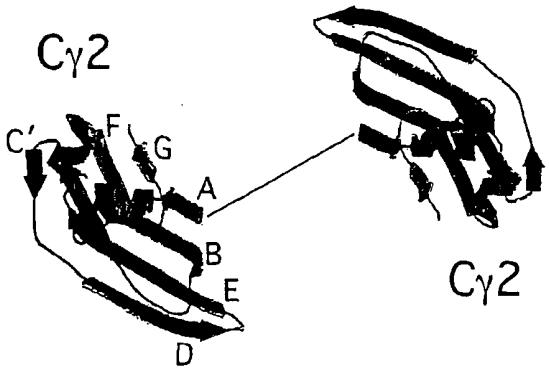


Fig. 2c

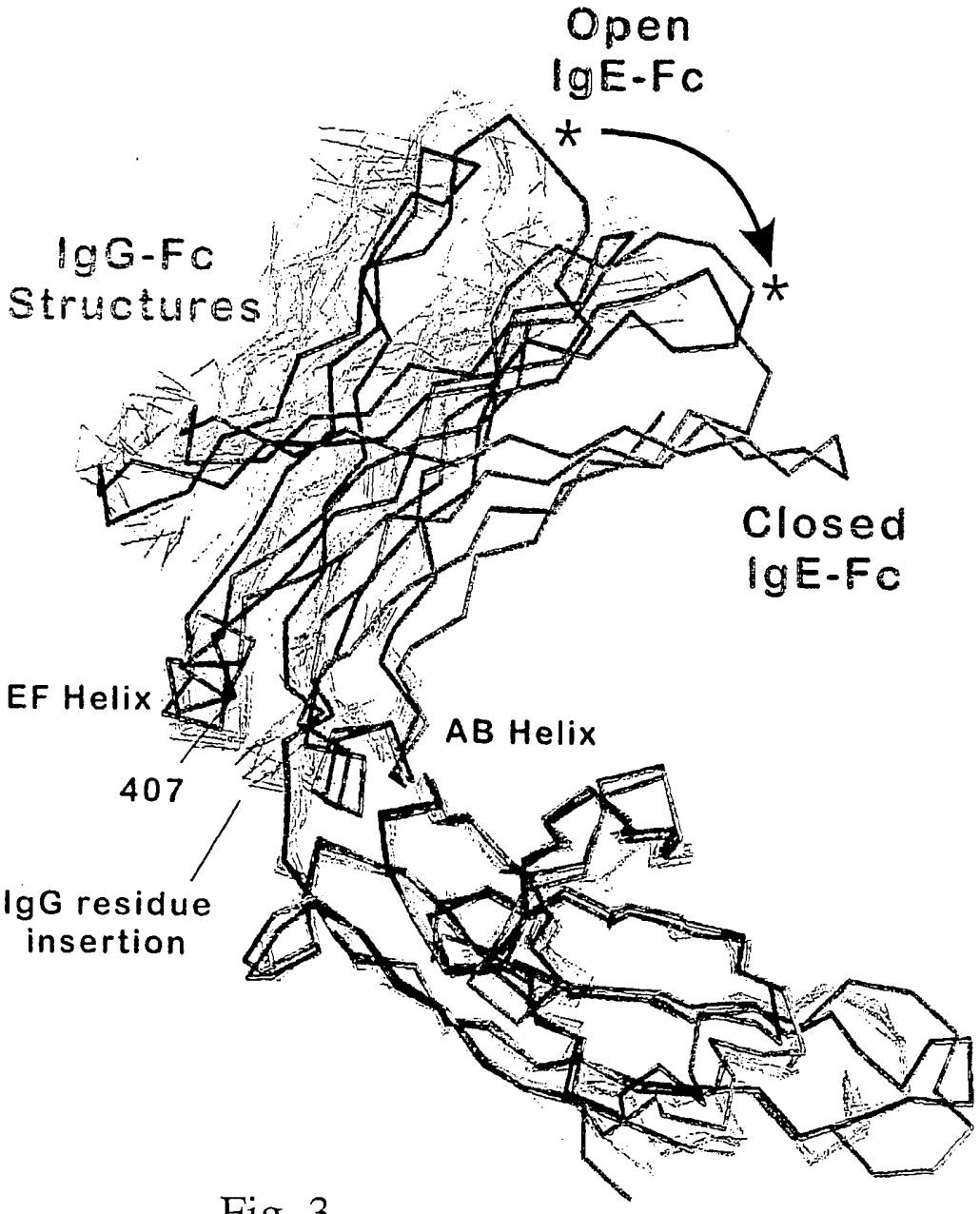


Fig. 3

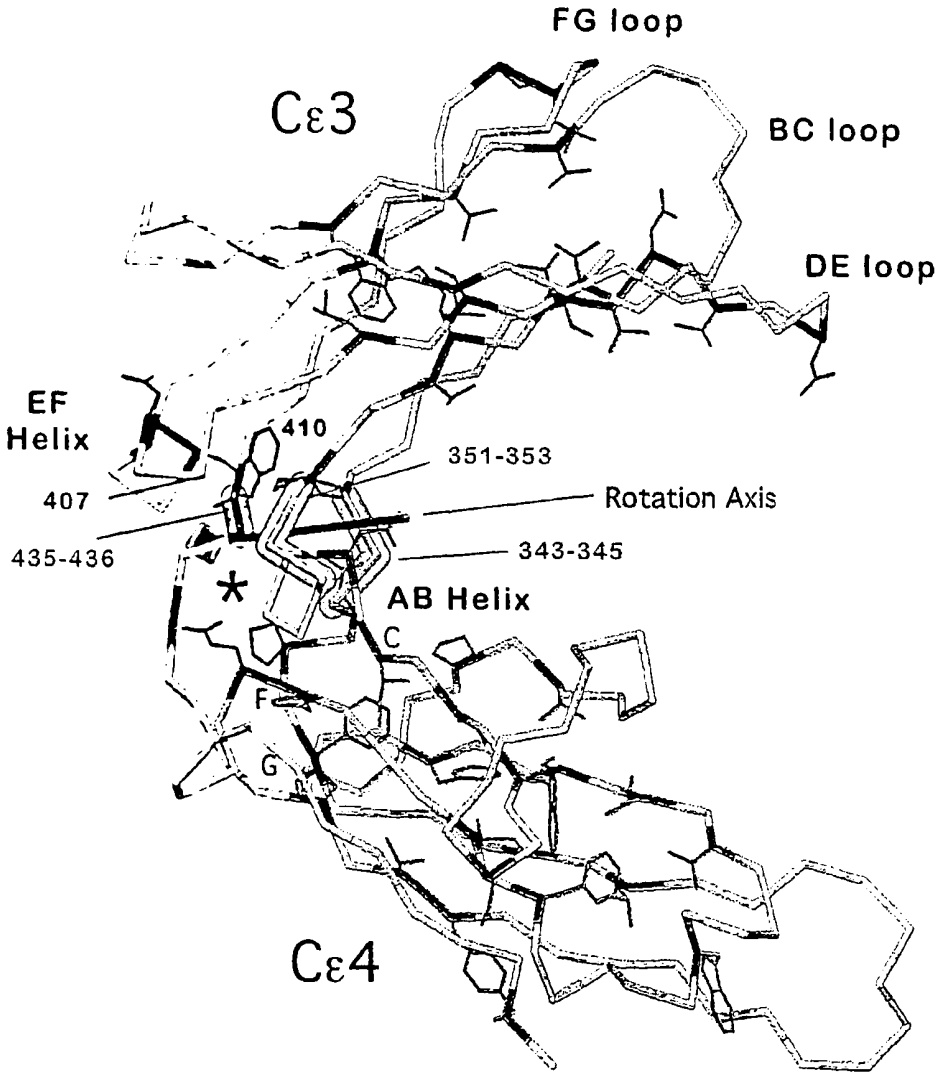


Fig. 4a

Fig. 4b

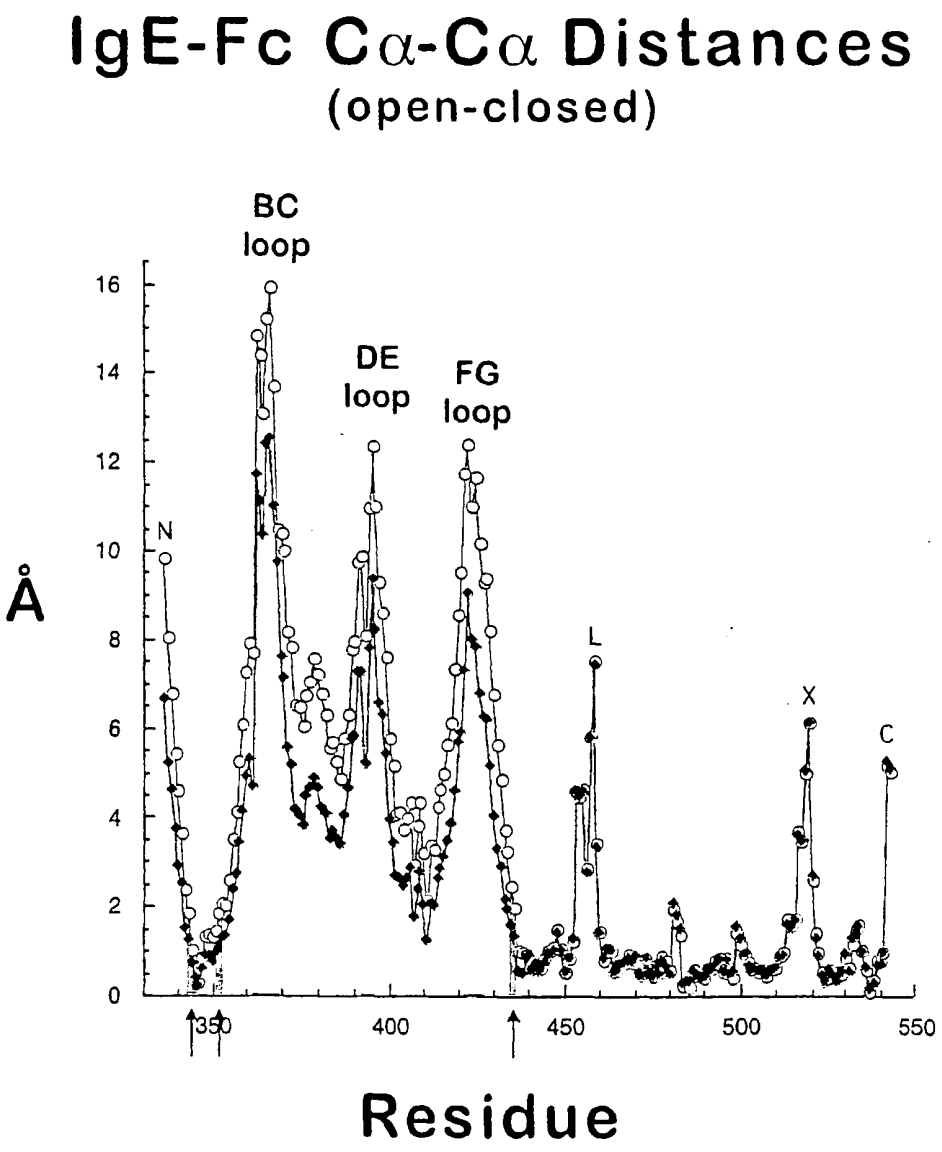


Fig. 4c

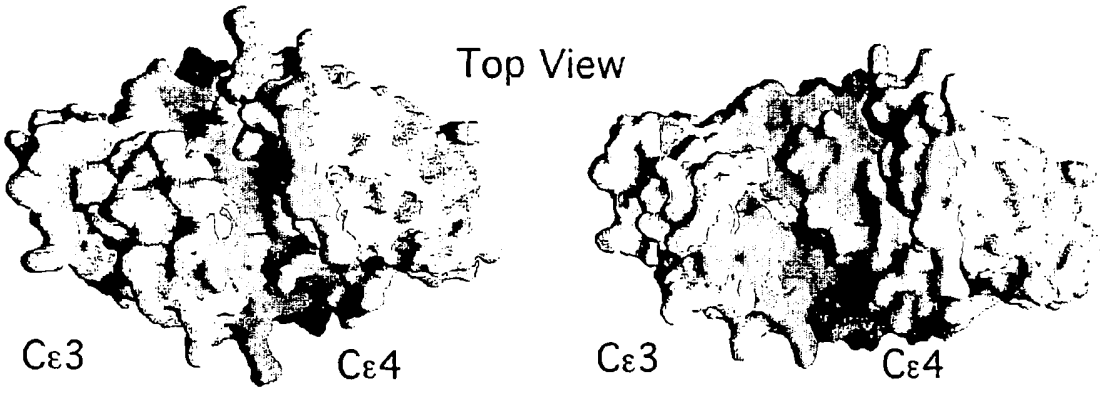


Fig. 5a

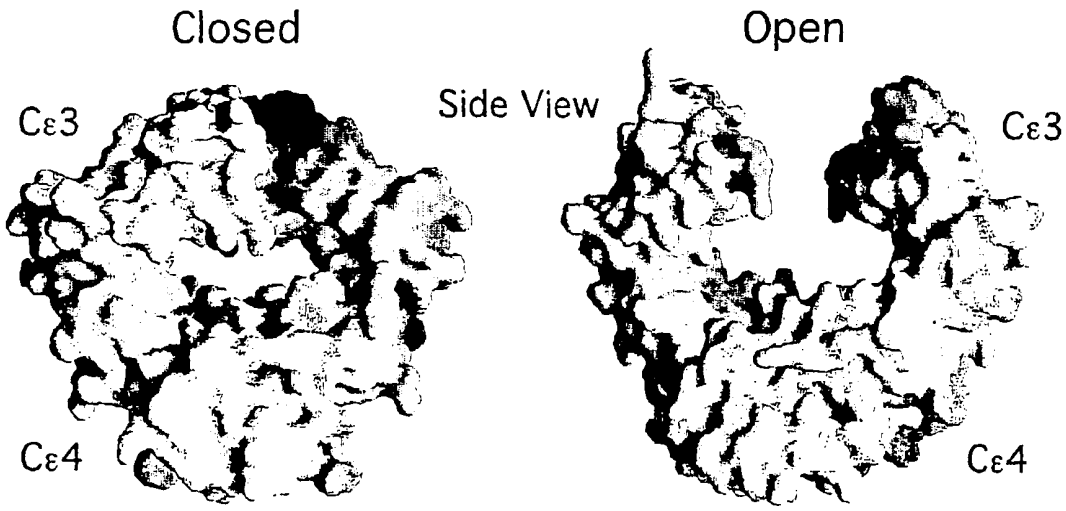


Fig. 5b

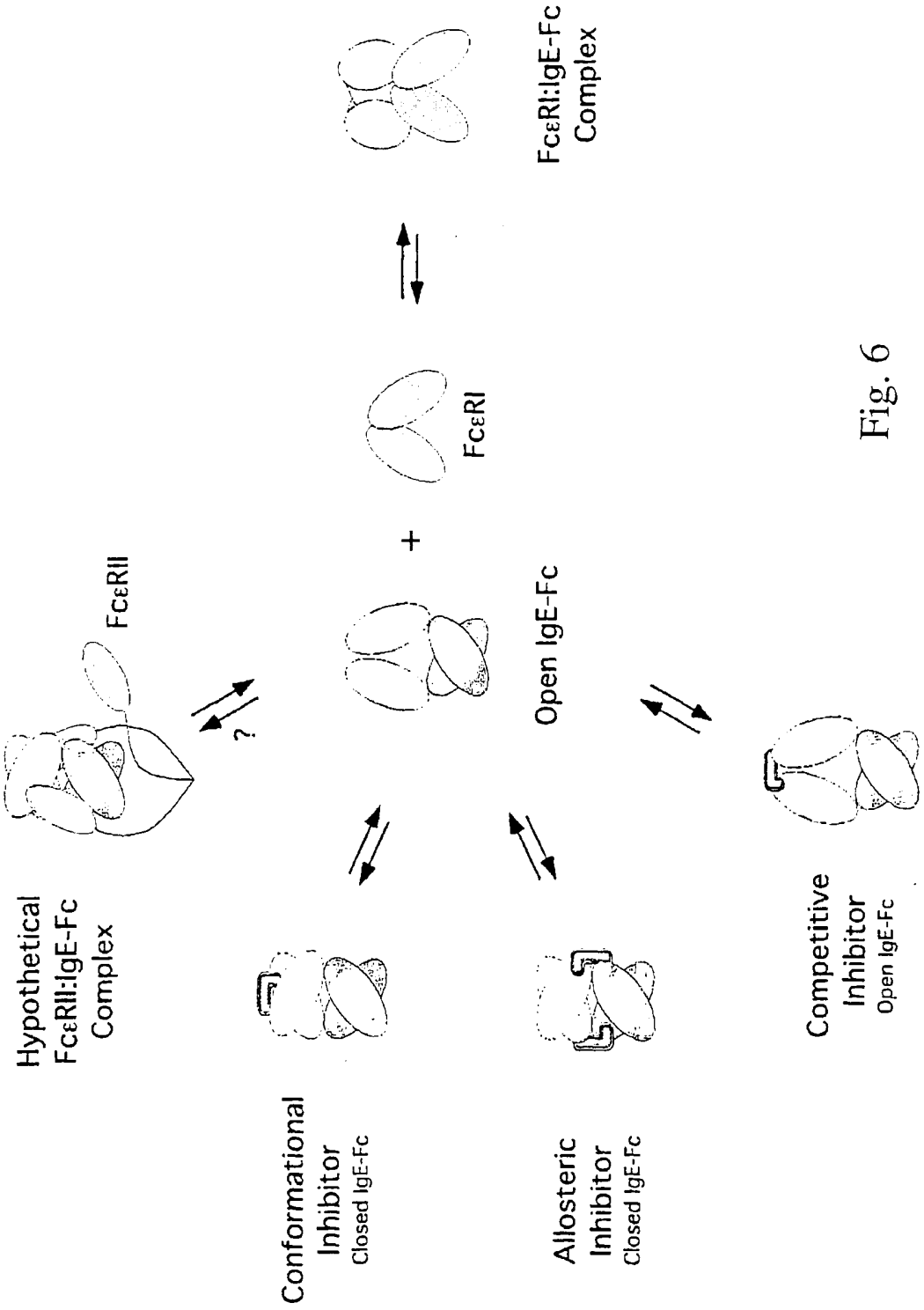


Fig. 6

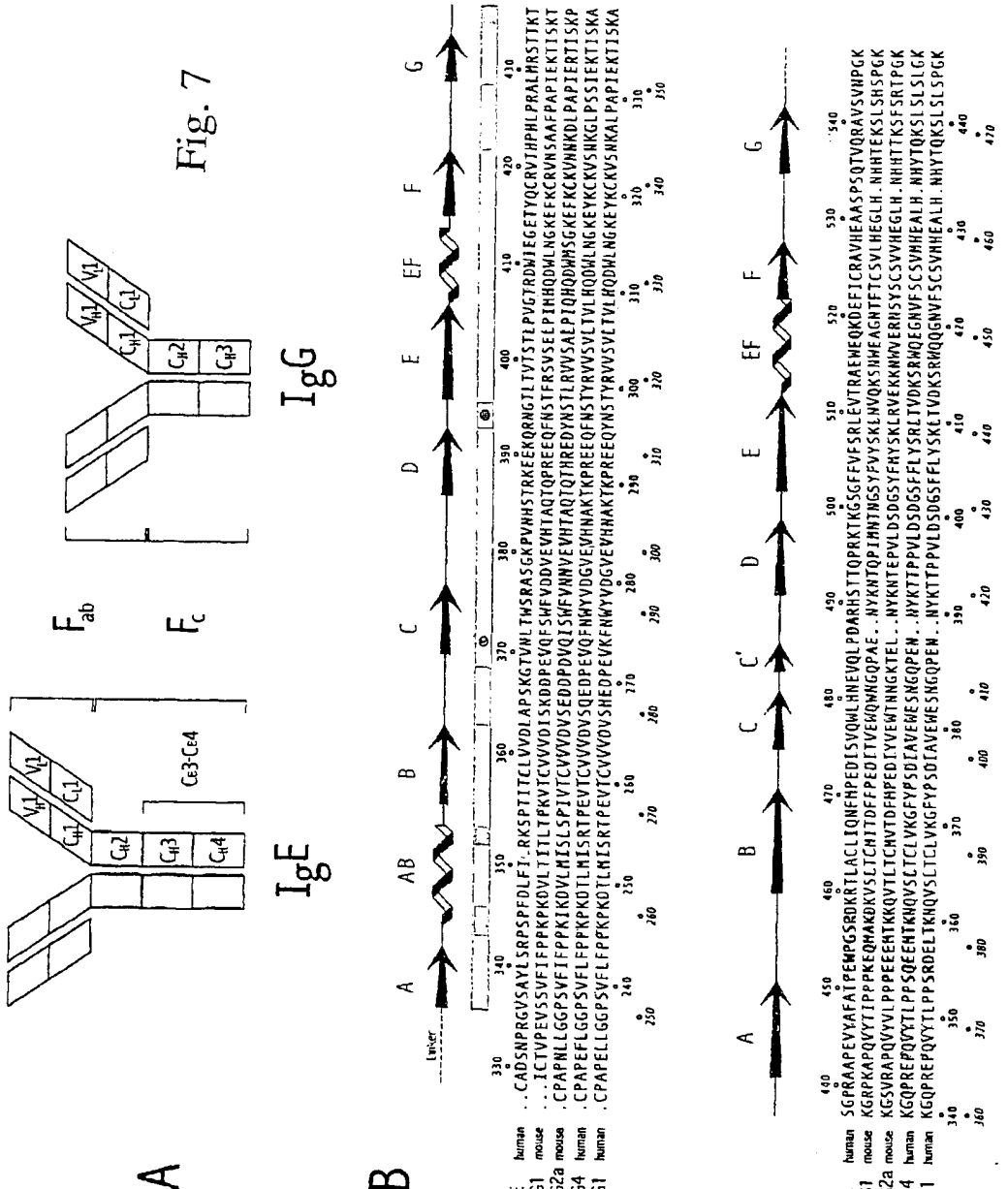


Fig. 7

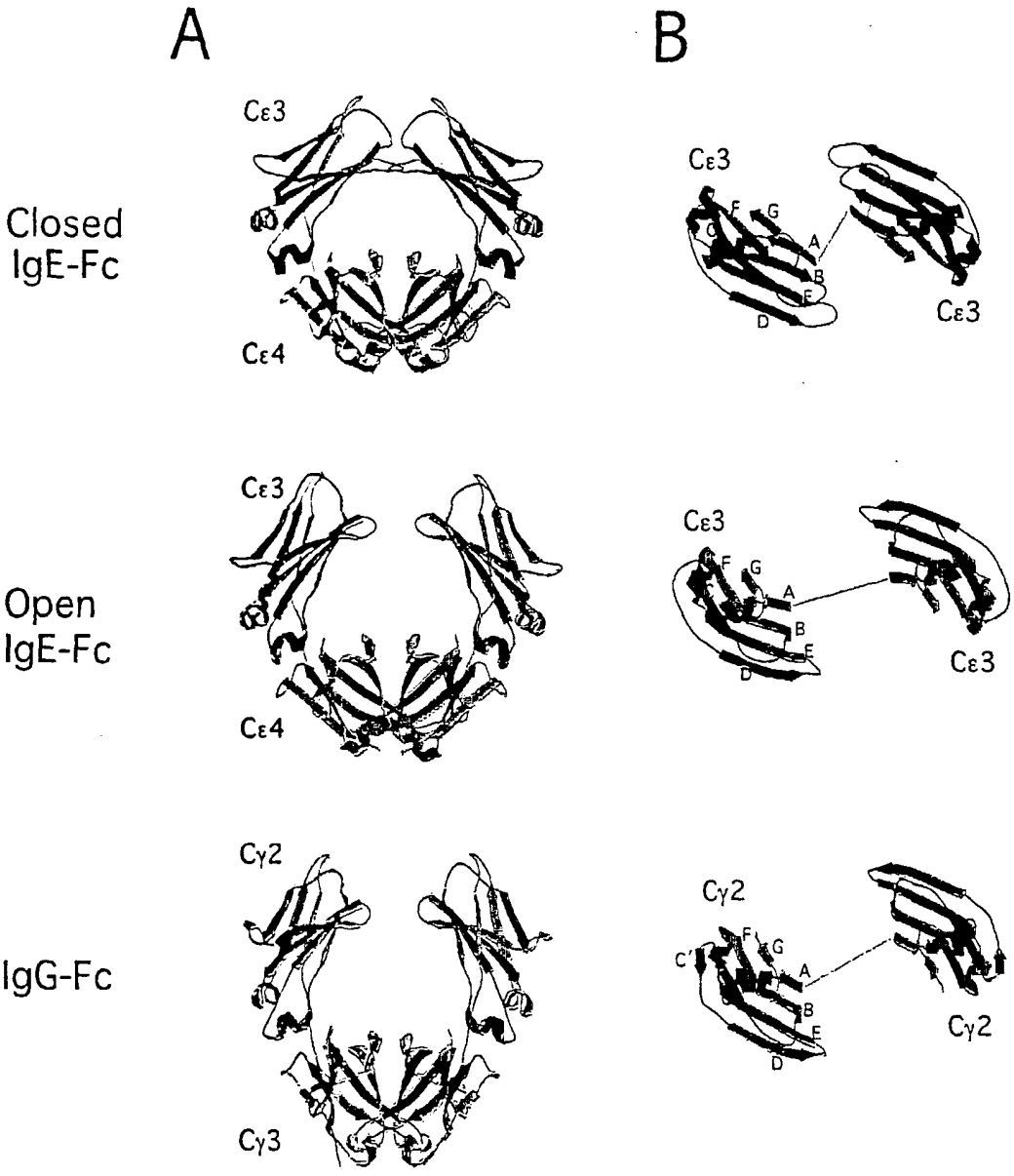


Fig. 8

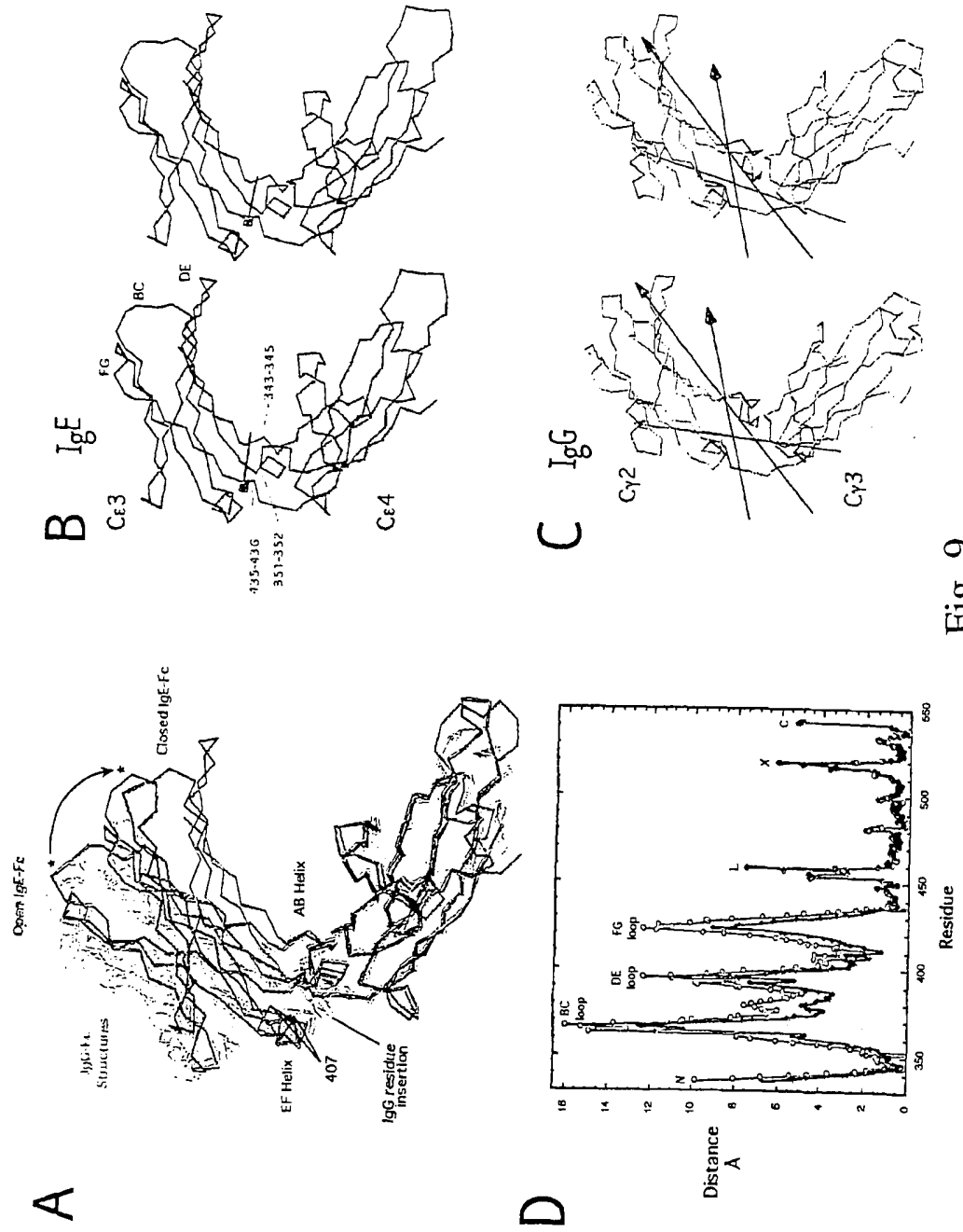


Fig. 9

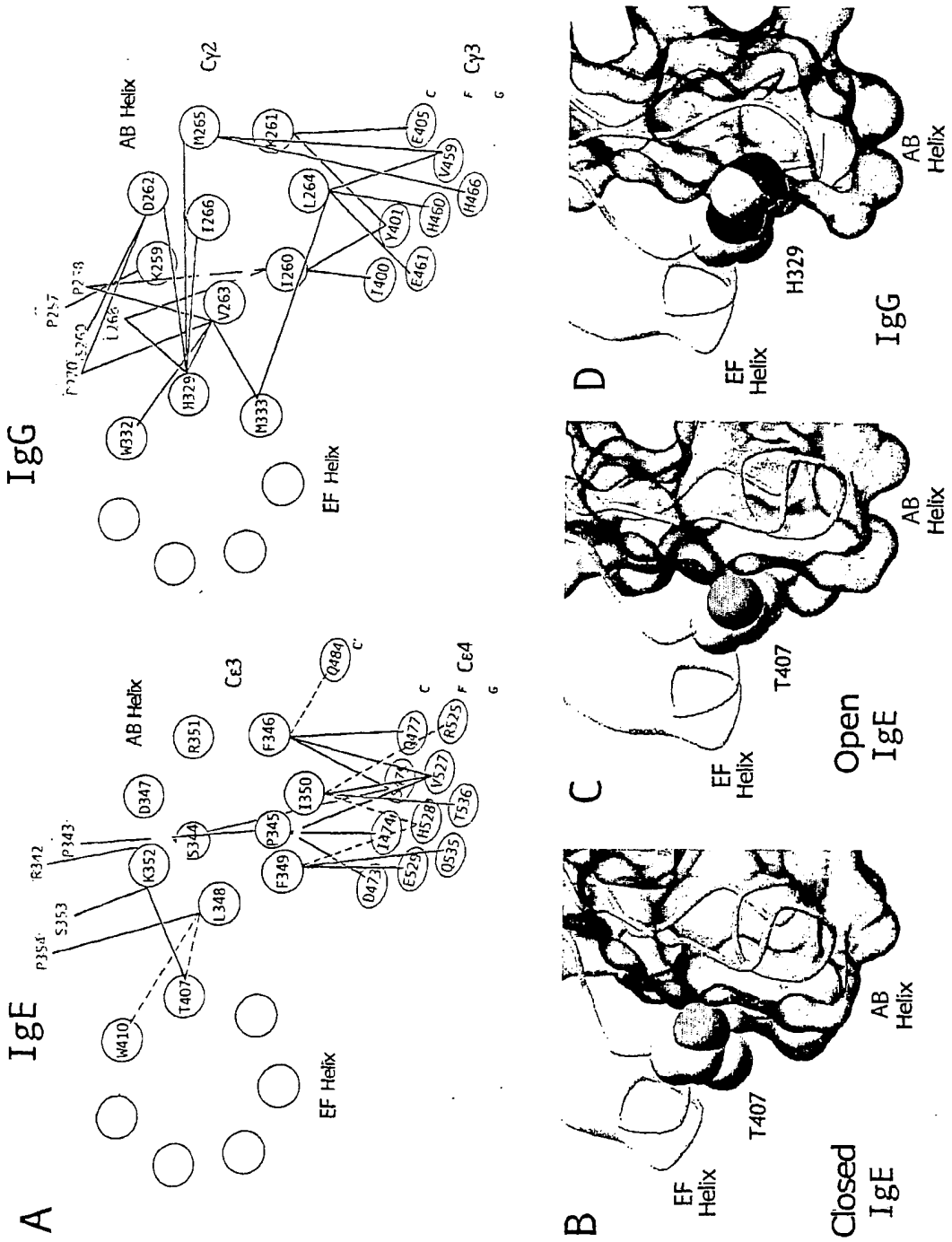


Fig. 10

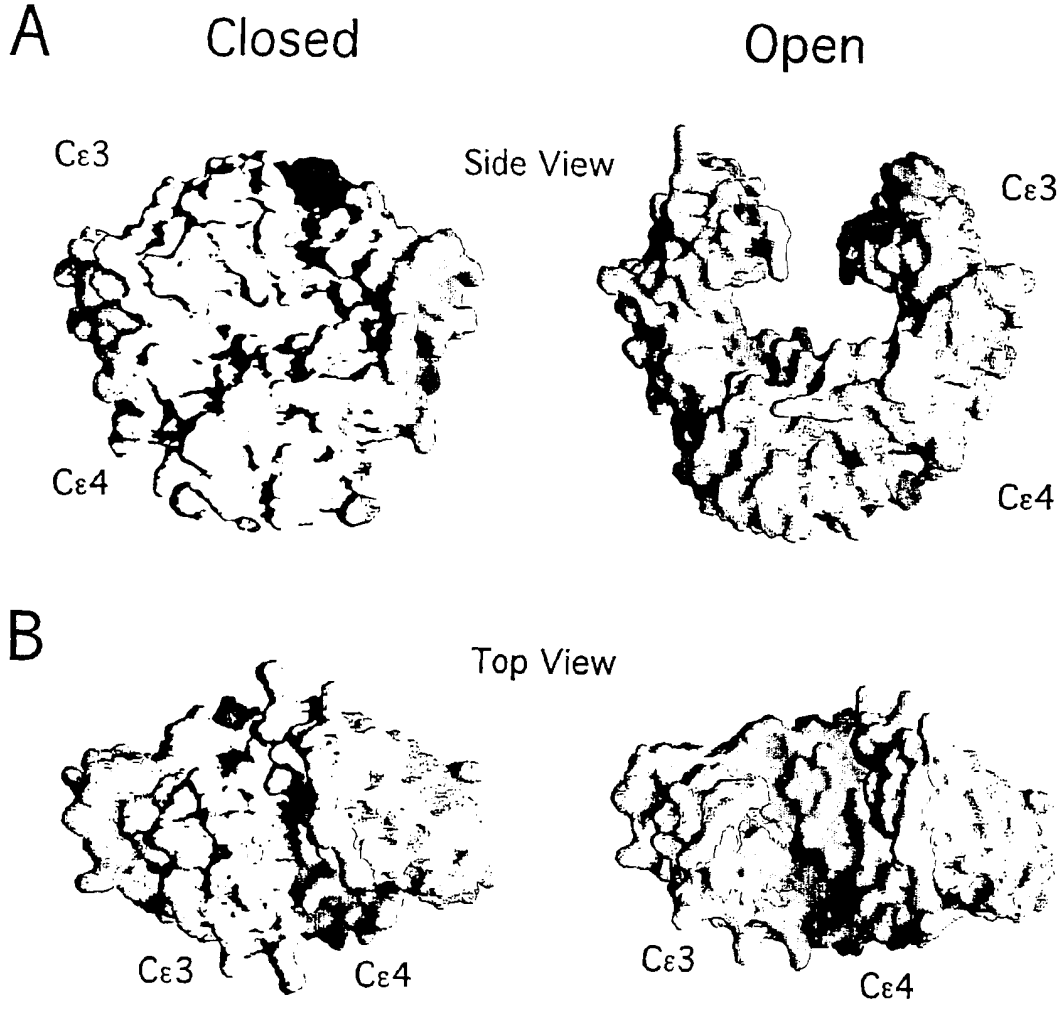


Fig. 11

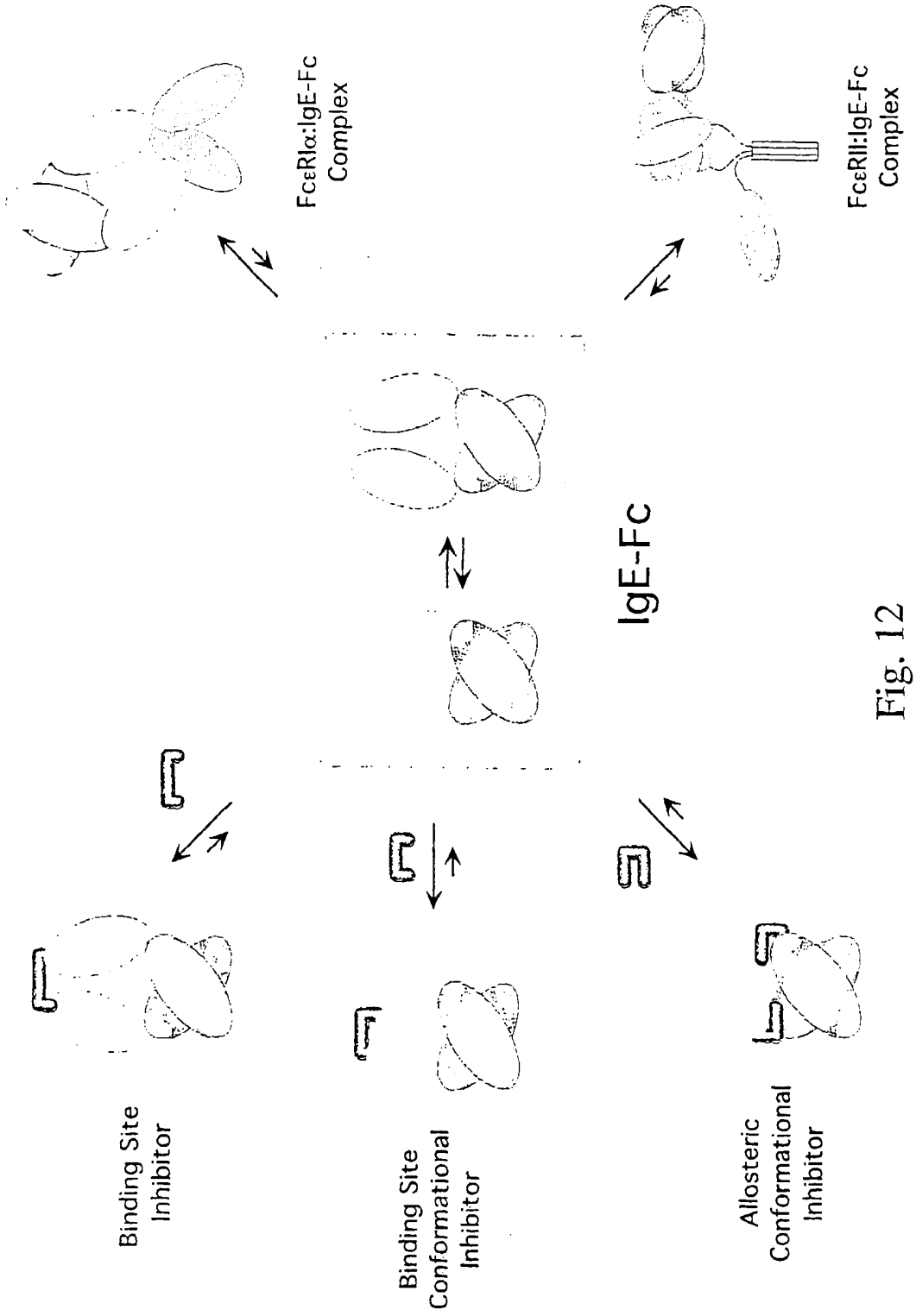
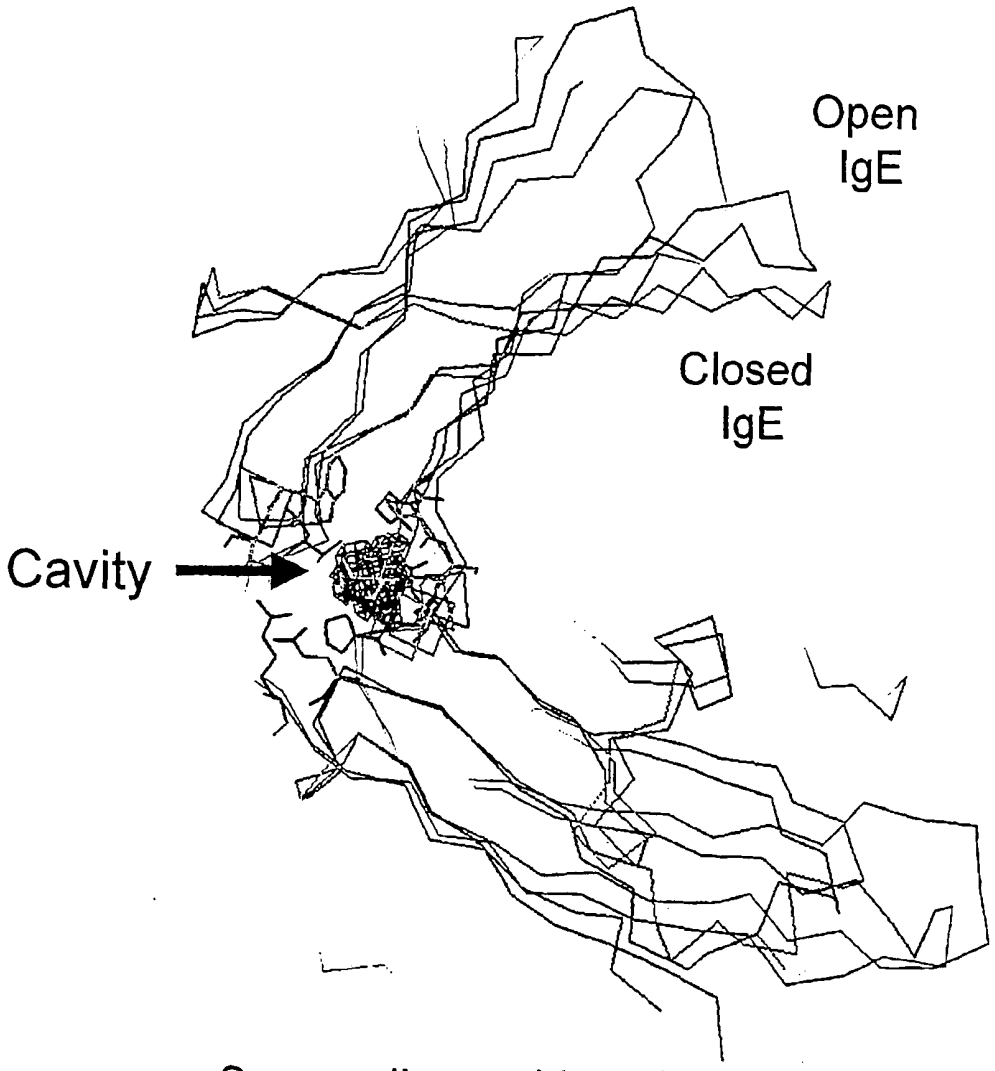


Fig. 12

A Potential Drug Binding Site Near the IgE-Fc Hinge



Surrounding residues include:
R342, P343, S344, P345, L348, W410, I411,
K435, T436, R440, P471, E472, D473, E529

Fig. 13

SEQUENCE LISTING

<110> Jardetzky, Theodore S.
Wurzburg, Beth A.

<120> THREE-DIMENSIONAL MODEL OF A Fc REGION OF AN IgE ANTIBODY AND USES THEREOF

<130> AL-9-C2-PCT

<140> not yet assigned
<141> 2001-03-15

<150> 60/234,877
<151> 2000-09-22

<150> 60/189,403
<151> 2000-03-15

<160> 2

<170> PatentIn Ver. 2.1

<210> 1
<211> 669
<212> DNA
<213> Homo sapiens

<220>
<221> CDS
<222> (1)..(666)

<400> 1

```
gcg gat ccc tgt gat tcc aac ccg aga ggg gtg agc gcc tac cta agc   48
Ala Asp Pro Cys Asp Ser Asn Pro Arg Gly Val Ser Ala Tyr Leu Ser
  1               5                  10                  15

cgg ccc agc ccg ttc gac ctg ttc atc cgc aag tcg ccc acg atc acc   96
Arg Pro Ser Pro Phe Asp Leu Phe Ile Arg Lys Ser Pro Thr Ile Thr
             20                  25                  30

tgt ctg gtg gtg gac ctg gca ccc agc aag ggg acc gtg aac ctg acc   144
Cys Leu Val Val Asp Leu Ala Pro Ser Lys Gly Thr Val Asn Leu Thr
         35                  40                  45

tgg tcc cgg gcc agt ggg aag cct gtg aac cac tcc acc aga aag gag   192
Trp Ser Arg Ala Ser Gly Lys Pro Val Asn His Ser Thr Arg Lys Glu
     50                  55                  60
```

```
gag aag cag cgc aat ggc acg tta acc gtc acg tcc acc ctg ccg gtg   240
Glu Lys Gln Arg Asn Gly Thr Leu Thr Val Thr Ser Thr Leu Pro Val
 65                  70                  75                  80

ggc acc cga gac tgg atc gag ggg gag acc tac cag tgc agg gtg acc   288
Gly Thr Arg Asp Trp Ile Glu Gly Glu Thr Tyr Gln Cys Arg Val Thr
                85                  90                  95

cac ccc cac ctg ccc agg gcc ctc atg cgg tcc acg acc aag acc agc   336
His Pro His Leu Pro Arg Ala Leu Met Arg Ser Thr Thr Lys Thr Ser
            100                 105                 110

ggc ccg cgt gct gcc ccg gaa gtc tat gcg ttt gcg acg ccg gag tgg   384
Gly Pro Arg Ala Ala Pro Glu Val Tyr Ala Phe Ala Thr Pro Glu Trp
        115                 120                 125

ccg ggg agc cgg gac aag cgc acc ctc gcc tgc ctg atc cag aac ttc   432
Pro Gly Ser Arg Asp Lys Arg Thr Leu Ala Cys Leu Ile Gln Asn Phe
    130                 135                 140

atg cct gag gac atc tcg gtg cag tgg ctg cac aac gag gtg cag ctc   480
Met Pro Glu Asp Ile Ser Val Gln Trp Leu His Asn Glu Val Gln Leu
145                 150                 155                 160

ccg gac gcc cgg cac agc acg acg cag ccc cgc aag acc aag ggc tcc   528
Pro Asp Ala Arg His Ser Thr Thr Gln Pro Arg Lys Thr Lys Gly Ser
                165                 170                 175

ggc ttc ttc gtc ttc agc cgc ctg gag gtg acc agg gcc gaa tgg gag   576
Gly Phe Phe Val Phe Ser Arg Leu Glu Val Thr Arg Ala Glu Trp Glu
            180                 185                 190

cag aaa gat gag ttc atc tgc cgt gca gtc cat gag gca gcg agc ccc   624
Gln Lys Asp Glu Phe Ile Cys Arg Ala Val His Glu Ala Ala Ser Pro
        195                 200                 205

tca cag acc gtc cag cga gcg gtg tct gta aat ccc ggt aaa tga       669
Ser Gln Thr Val Gln Arg Ala Val Ser Val Asn Pro Gly Lys
    210                 215                 220
```

<210> 2
<211> 222
<212> PRT
<213> Homo sapiens

<400> 2

```
Ala Asp Pro Cys Asp Ser Asn Pro Arg Gly Val Ser Ala Tyr Leu Ser
 1               5                  10                  15

Arg Pro Ser Pro Phe Asp Leu Phe Ile Arg Lys Ser Pro Thr Ile Thr
            20                  25                  30

Cys Leu Val Val Asp Leu Ala Pro Ser Lys Gly Thr Val Asn Leu Thr
        35                  40                  45

Trp Ser Arg Ala Ser Gly Lys Pro Val Asn His Ser Thr Arg Lys Glu
    50                  55                  60

Glu Lys Gln Arg Asn Gly Thr Leu Thr Val Thr Ser Thr Leu Pro Val
65                  70                  75                  80

Gly Thr Arg Asp Trp Ile Glu Gly Glu Thr Tyr Gln Cys Arg Val Thr
                85                  90                  95

His Pro His Leu Pro Arg Ala Leu Met Arg Ser Thr Thr Lys Thr Ser
            100                 105                 110

Gly Pro Arg Ala Ala Pro Glu Val Tyr Ala Phe Ala Thr Pro Glu Trp
        115                 120                 125

Pro Gly Ser Arg Asp Lys Arg Thr Leu Ala Cys Leu Ile Gln Asn Phe
    130                 135                 140

Met Pro Glu Asp Ile Ser Val Gln Trp Leu His Asn Glu Val Gln Leu
145                 150                 155                 160

Pro Asp Ala Arg His Ser Thr Thr Gln Pro Arg Lys Thr Lys Gly Ser
                165                 170                 175

Gly Phe Phe Val Phe Ser Arg Leu Glu Val Thr Arg Ala Glu Trp Glu
            180                 185                 190

Gln Lys Asp Glu Phe Ile Cys Arg Ala Val His Glu Ala Ala Ser Pro
        195                 200                 205

Ser Gln Thr Val Gln Arg Ala Val Ser Val Asn Pro Gly Lys
    210                 215                 220
```

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
20 September 2001 (20.09.2001)

PCT

(10) International Publication Number
WO 01/68861 A3

(51) International Patent Classification[7]: C12N 15/13, C07K 16/00, C12N 15/86, 5/10, G01N 33/53, A61P 37/08, A61K 39/395, 31/00

(21) International Application Number: PCT/US01/08523

(22) International Filing Date: 15 March 2001 (15.03.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:

60/189,403	15 March 2000 (15.03.2000)	US
60/234,877	22 September 2000 (22.09.2000)	US

(71) Applicant *(for all designated States except US)*: **NORTHWESTERN UNIVERSITY** [US/US]; 633 Clark Street, Evanston, IL 60201 (US).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **JARDETZKY, Theodore, S.** [US/US]; 7518 N. Eastlake Terrace, Chicago, IL 60626 (US). **WURZBURG, Beth, A.** [US/US]; 2544 Prairie Ave., No 33, Evanston, IL 60201 (US).

(74) Agents: **VERSER, Carol, Talkington** et al.; Heska Corporation, 1613 Prospect Parkway, Fort Collins, CO 80525 (US).

(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report*

(88) Date of publication of the international search report:
21 March 2002

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

WO 01/68861 A3

(54) Title: THREE-DIMENSIONAL MODEL OF A Fc REGION OF AN IgE ANTIBODY AND USES THEREOF

(57) Abstract: The present invention includes three-dimensional models of antibodies, such as Fc-Cε3/Cε4 regions of IgE antibodies, as well as methods to produce such models. The present invention also includes muteins having increased stabiltiy and/or antibody receptor binding activity, as well as methods to produce such muteins, preferably using information derived from three-dimensional models of the present invention. Also included are nucleic acid sequences encoding muteins of the present invention and use of those sequences to produce such muteins. Also included is the use of themodel to identify compounds that inhibit the binding of an antibody receptor protein to an antibody. The present invention also includes uses of such muteins and inhibitory compounds, for example, in methods to diagnose and protect animals from allergy and othter abnormal immune responses.

INTERNATIONAL SEARCH REPORT

Int' tional Application No
PCT/US 01/08523

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C12N15/13 C07K16/00 C12N15/86 C12N5/10 G01N33/53
A61P37/08 A61K39/395 A61K31/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
BIOSIS, EMBASE, WPI Data, PAJ, EPO-Internal

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 95 14779 A (RESEARCH EXPLOITATION LIMITED) 1 June 1995 (1995-06-01) claims seq. id. no. 1 figure 1 ---	37, 39-41, 43,44
A	E. PADLAN ET AL.: "A model of the Fc of immunoglobulin E." MOLECULAR IMMUNOLOGY, vol. 23, no. 10, October 1986 (1986-10), pages 1063-1075, XP001041593 Oxford, GB abstract page 1074, left-hand column, line 48 -right-hand column, line 16 --- -/--	1-69

[X] Further documents are listed in the continuation of box C.

[X] Patent family members are listed in annex

° Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
3 December 2001	20/12/2001

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Nooij, F

2

Form PCT/ISA/210 (second sheet) (July 1992)

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication where appropriate, of the relevant passages	Relevant to claim No.
A	L. PRESTA ET AL.: "The binding site on human immunoglobulin E for its high affinity receptor." THE JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 269, no. 42, 21 October 1994 (1994-10-21), pages 26368-26373, XP002184546 Baltimore, MD, USA the whole document	1-69
A	M. VERNERSSON ET AL.: "Cloning, structural analysis, and expression of the pig IgE epsilon chain." IMMUNOGENETICS, vol. 46, no. 6, 1997, pages 461-468, XP002184547 abstract	1-69
A	I. SAYERS ET AL.: "Amino acid residues that influence FcepsilonRI-mediated effector functions of human immunoglobulin E." BIOCHEMISTRY, vol. 37, no. 46, 17 November 1998 (1998-11-17), pages 16152-16164, XP002184548 Washington, DC, USA abstract page 16163, right-hand column, line 17 - line 23	1-69
A	A. BEAVIL ET AL.: "Automated hydrodynamic modelling of a complex between a human IgE fragment (Fcepsilon3-4) and the IgE high affinity receptor FcepsilonRI alpha-chain." EUROPEAN BIOPHYSICS JOURNAL, vol. 25, no. 5-6, 1997, pages 463-469, XP000905144 abstract	1-69
P,X	B. WURZBURG ET AL.: "Structure of the human IgE-Fc Cepsilon3-Cepsilon4 reveals conformational flexibility in the antibody effector domains." IMMUNITY, vol. 13, no. 3, September 2000 (2000-09), pages 375-385, XP002184549 the whole document	1-69
P,A	WO 00 26246 A (HESKA CORPORATION ET AL.) 11 May 2000 (2000-05-11) the whole document	1-69

2

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 1-25,45-69 (all partially)

Present claims 1-25, 45-61, 65 and 66 relate to a 3-D model, and its use, characterized by technical features which, also due to the use of the word "substantially", do not allow a complete search for this subject as being not completely defined.
Further, present claims 65-69 relate to or comprise compounds or their use defined by reference to a desirable characteristic or property:
According to the description, the isolated IgE Fc-region comprising Cepsilon3 and Cepsilon4 domains, upon which the crystal has been based, is represented by SEQ. ID. No. 2 (see page 12, lines 9-16), muteins thereof have only be defined by desired properties or DNA coding therefor.
The claims cover all compounds having this characteristic or property, whereas the application provides support within the meaning of Article 6 PCT and/or disclosure within the meaning of Article 5 PCT for only a very limited number of such compounds (see claim 37 and the examples). In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT).
An attempt is made to define compounds by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible.
Furthermore, the claims 62-64 relate to or encompass compounds that have only been defined by their ability to inhibit the binding between an IgE antibody and a FcepsilonRIalpha protein. The same objections under Art. 6 PCT are also applicable, mutatis mutandis, to the claims 62-64.
Consequently, the search has been carried out for those parts of the claims which appear to be clear, supported and disclosed, namely those parts relating to the compounds defined in claim 37, that is the compounds having the SEQ. ID. No. 2 and crystals of said compunds.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

INTERNATIONAL SEARCH REPORT

Information on patent family members

Intr ational Application No
PCT/US 01/08523

Patent document cited in search report		Publication date	Patent family member(s)		Publication date
WO 9514779	A	01-06-1995	AU	1072395 A	13-06-1995
			EP	0730649 A1	11-09-1996
			WO	9514779 A1	01-06-1995
WO 0026246	A	11-05-2000	AU	1909500 A	22-05-2000
			EP	1127076 A2	29-08-2001
			WO	0026246 A2	11-05-2000

Form PCT/ISA/210 (patent family annex) (July 1992)